

High Throughput Quantitative Analysis

MassHunter Quantitative Analysis Webinar Series

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MassHunter Quantitative Analysis Software

Review and Quant Method Optimization

What is quantitative analysis?

In analytical chemistry, quantitative analysis is the determination of the absolute or relative abundance (often expressed as a concentration) of one, several or all particular substance(s) present in a sample.

From [https://en.wikipedia.org/wiki/Quantitative_analysis_\(chemistry\)](https://en.wikipedia.org/wiki/Quantitative_analysis_(chemistry))

Quantitative chemical analysis, branch of chemistry that deals with the determination of the amount or percentage of one or more constituents of a sample.

From <https://www.britannica.com/science/quantitative-chemical-analysis>

Quantitative analysis refers to the determination of how much of a given component is present in a sample.

From <https://www.thoughtco.com/definition-of-quantitative-analysis-604627>

How do I know that the compound that is identified is indeed the correct compound?'

Target Compound Analysis

Retention Time

- A given compound will come out at a specified time under a given set of chromatographic conditions.
- Dual column analysis with columns of different polarities.

Target Ion

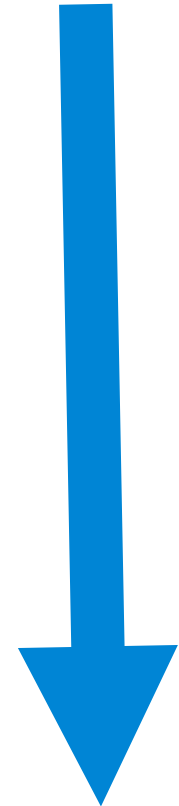
- Must be unique to the compound of interest in the time range of interest.

Qualifier Ions

- Must be present in the same specified time range.
- Must be present in specific ratios relative to the Target Ion.

Target and Qualifiers

- Must be within the given correlation window.
- Should maintain similar peak shapes.



Increasing Confidence

Analysts are buried in data!!!

Analysts are being overwhelmed with data ... hundreds of compounds... multiple signals per compound... 10's or even hundreds of samples in a batch.

Add an initial calibration, a continuing calibration or a QC and other data review functions and the analyst is overwhelmed with data.

Chromatographic runs are shorter; thus more data in a given period of time.

What can what can MassHunter Quantitative Analysis software do to help?



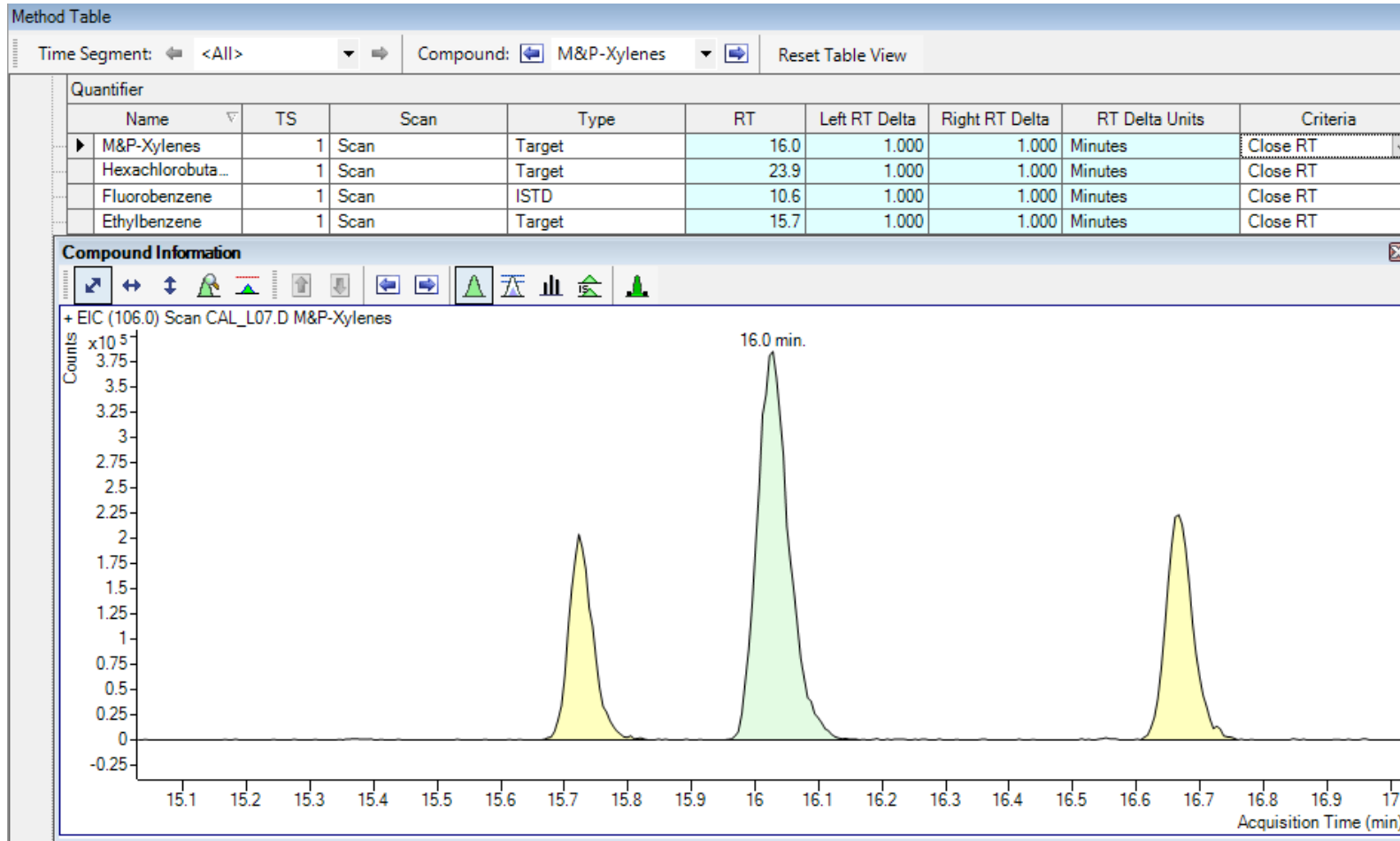
Quant Method Check List

- Extract the compounds signals in the correct RT Window.
- Utilize the correct integrator and settings for each compound.
- Reduce unwanted peaks with
 - Reference and Non Reference Windows
 - Integration parameters
 - Peak Filters
 - Peak Filter Area Threshold
 - Zero Peaks Below LOD
 - Correlation Window
- Updating Retention Time Drift
- Retention Times
- Qualifier Ion Ratios
- Update Mass Assignments

Objective is to intelligently minimize the number of compounds that require review.

Retention Time Setup

RT Delta



Left and Right RT Delta determines the time range over which the specified signal is extracted.

RT Delta Units

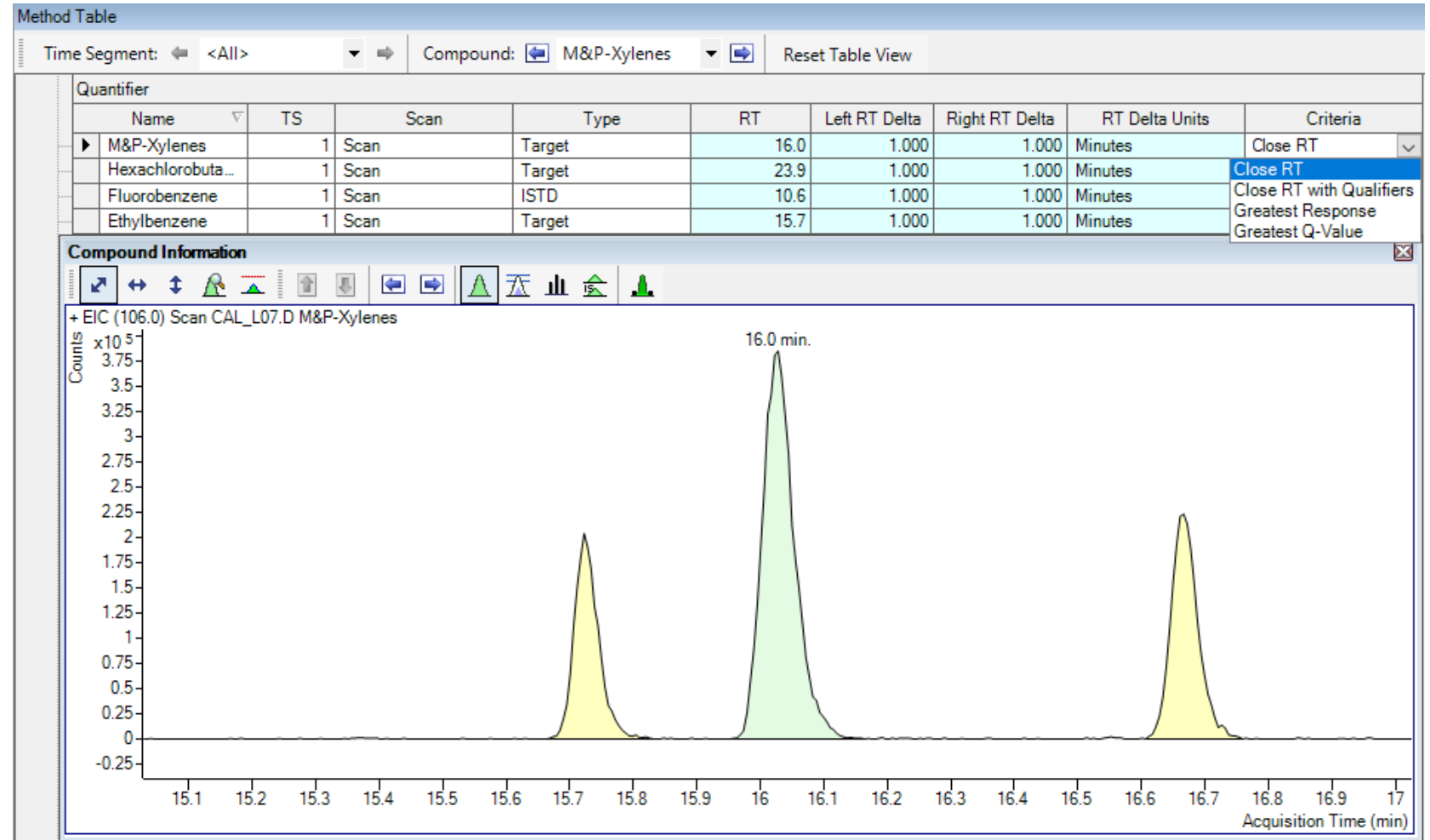
- **Percent** – Uses a percentage of RT, good for long runs where retention time shifts can be larger late in the run.
- **Minutes** - Absolute minutes.

Default is 1 minute. A narrower window can be setup if needed.

Retention Time Setup Criteria

When multiple peaks are found in RT window, Criteria decides which peak to use.

- Close RT
- Close RT with Qualifiers
- Greatest Response
- Greatest Q-Value



Reference & Non Reference Window Definitions

Defined in Globals Setup in the Method Editor

Reference Window

- Applies only to compounds labeled as Time Reference.
- Only ISTDs can be labeled as Time Reference.
- Algorithm looks for ISTDs first, then target compounds related to that ISTD.

Non Reference Window

- Applies to all other compounds.

Recognition and Reference Windows are synonymous terms.

The screenshot displays the Agilent Method Editor interface. On the left, the 'Method Tasks' sidebar is visible, with 'Globals Setup' highlighted in a red box. The main window shows the 'Method Table' with a 'Sample' table and a 'Globals' configuration table.

| Name | Data File | Type | Level | Acq. Method File |
|---------|--------------|-------|-------|------------------|
| Blank-1 | CMAMBIk_01.d | Blank | | APC\autotune.m |

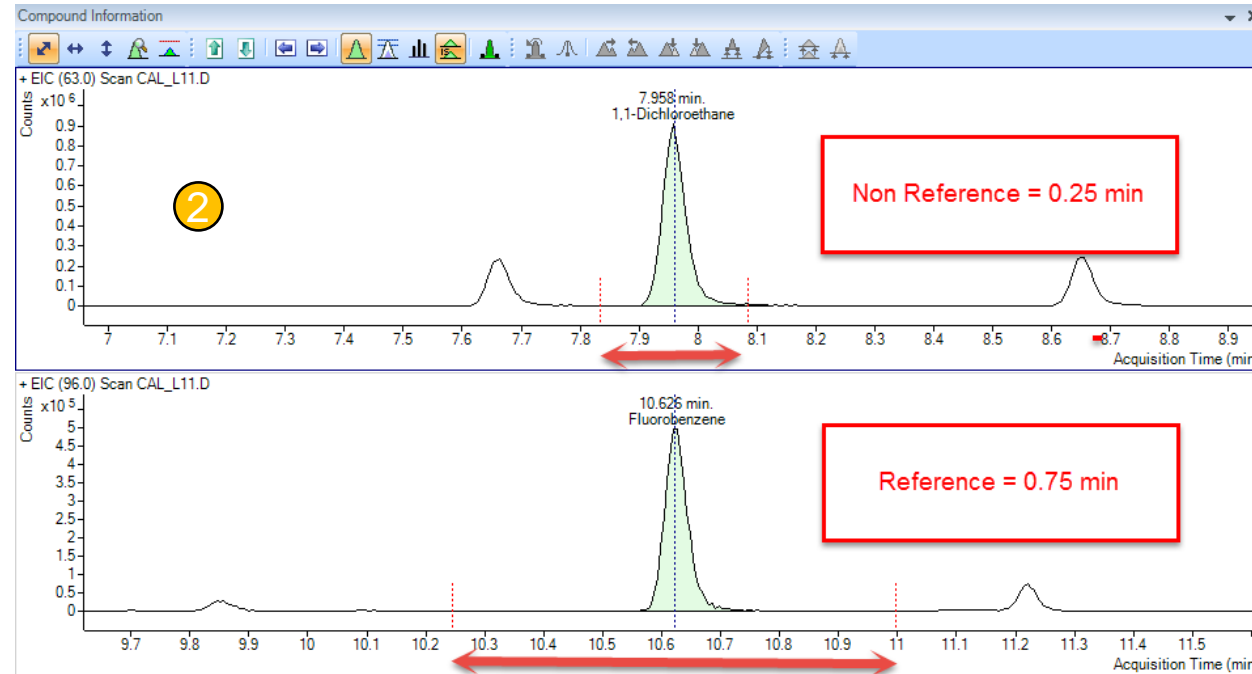
| Globals | |
|----------------------------------|-------------------------------------|
| Apply Multiplier to ISTD | <input type="checkbox"/> |
| Apply Multiplier to Matrix Spike | <input checked="" type="checkbox"/> |
| Apply Multiplier to Surrogate | <input checked="" type="checkbox"/> |
| Apply Multiplier to Target | <input checked="" type="checkbox"/> |
| Bracketing Type | None |
| Correlation Window | 2.000 |
| Dynamic Background Subtraction | <input type="checkbox"/> |
| Ignore Peaks Not Found | <input type="checkbox"/> |
| Library Method | |
| Non Reference Window | 200.000 |
| Non Reference Window Type | Percent |
| Reference Library | |
| Reference Pattern Library | |
| Reference Window | 80.000 |
| Reference Window Type | Percent |
| Relative ISTD | <input type="checkbox"/> |
| Standard Addition | <input type="checkbox"/> |

Reference & Non Reference Window

1

| Globals | |
|----------------------------------|-------------------------------------|
| Apply Multiplier to ISTD | <input type="checkbox"/> |
| Apply Multiplier to Matrix Spike | <input checked="" type="checkbox"/> |
| Apply Multiplier to Surrogate | <input checked="" type="checkbox"/> |
| Apply Multiplier to Target | <input checked="" type="checkbox"/> |
| Bracketing Type | None |
| CC Maximum Elapsed Time In Hours | 0.000 |
| Correlation Window | 2.000 |
| Dynamic Background Subtraction | <input type="checkbox"/> |
| Ignore Peaks Not Found | <input type="checkbox"/> |
| Library Method | |
| Non Reference Window | 0.250 |
| Non Reference Window Type | Minutes |
| Reference Library | |
| Reference Pattern Library | |
| Reference Window | 0.750 |
| Reference Window Type | Minutes |
| Relative ISTD | <input type="checkbox"/> |
| Standard Addition | <input type="checkbox"/> |

Restricts peak selection to a smaller RT window.



2

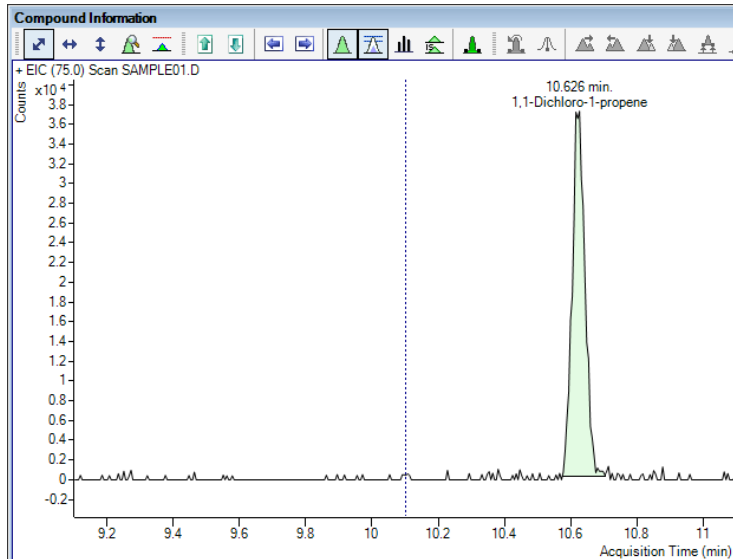
3

| Quantifier | | | | | | | | |
|------------|-------------------------|----|------|-----------|--------------------|-------------------------------------|------------|-------------------------------------|
| | Name | TS | Scan | Type | ISTD Compound Name | ISTD Flag | ISTD Conc. | Time Reference Flag |
| ▶ | Fluorobenzene | 1 | Scan | ISTD | <None> | <input checked="" type="checkbox"/> | 10.0000 | <input checked="" type="checkbox"/> |
| | Chlorobenzene-d5 | 1 | Scan | ISTD | <None> | <input checked="" type="checkbox"/> | 10.0000 | <input type="checkbox"/> |
| | 1,4-Dichlorobenzene-d4 | 1 | Scan | ISTD | <None> | <input checked="" type="checkbox"/> | 10.0000 | <input type="checkbox"/> |
| | 1,2-Dichloroethane-d4 | 1 | Scan | Surrogate | Fluorobenzene | <input type="checkbox"/> | 10.0000 | <input type="checkbox"/> |
| | Toluene-D8 | 1 | Scan | Surrogate | Chlorobenzene-d5 | <input type="checkbox"/> | 10.0000 | <input type="checkbox"/> |
| | 1,1-Dichloro-1-propene | 1 | Scan | Target | Fluorobenzene | <input type="checkbox"/> | 10.0000 | <input type="checkbox"/> |
| | Dichlorodifluoromethane | 1 | Scan | Target | Fluorobenzene | <input type="checkbox"/> | 10.0000 | <input type="checkbox"/> |
| | Chloromethane | 1 | Scan | Target | Fluorobenzene | <input type="checkbox"/> | 10.0000 | <input type="checkbox"/> |

Reference = ISTD + Time Reference

Non Reference = Everything else

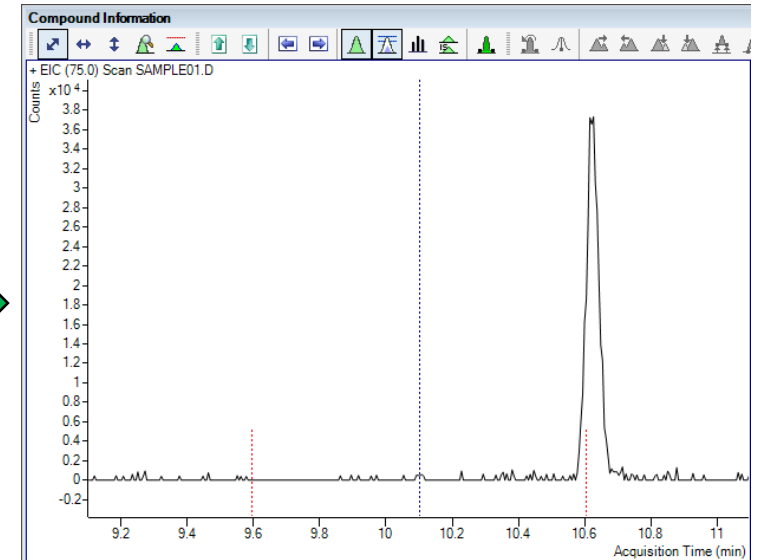
Non Reference Window



Initial Values

| Globals | |
|----------------------------------|-------------------------------------|
| Apply Multiplier to ISTD | <input type="checkbox"/> |
| Apply Multiplier to Matrix Spike | <input checked="" type="checkbox"/> |
| Apply Multiplier to Surrogate | <input checked="" type="checkbox"/> |
| Apply Multiplier to Target | <input checked="" type="checkbox"/> |
| Bracketing Type | None |
| Correlation Window | 2.000 |
| Dynamic Background Subtraction | <input type="checkbox"/> |
| Ignore Peaks Not Found | <input type="checkbox"/> |
| Library Method | |
| Non Reference Window | 10.000 |
| Non Reference Window Type | Percent |
| Reference Library | |
| Reference Pattern Library | |
| Reference Window | 80.000 |
| Reference Window Type | Percent |
| Relative ISTD | <input type="checkbox"/> |
| Standard Addition | <input type="checkbox"/> |

Adjusted Values

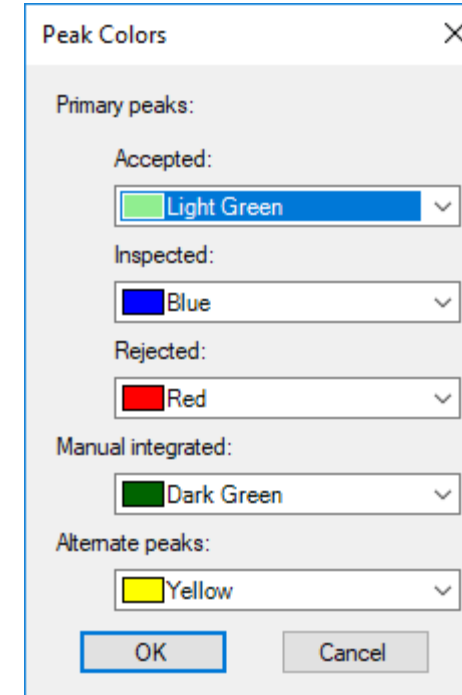
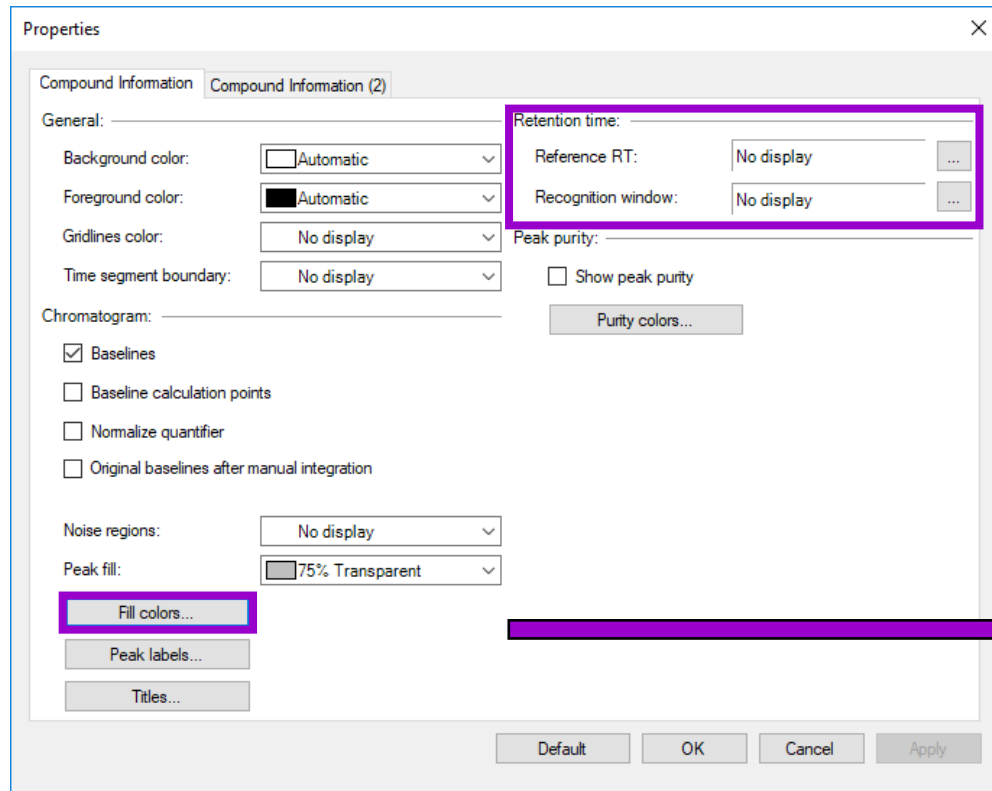


Final Values

Reduce the Non Reference Window from the default 200% to 10%. This helps eliminate false positives and reduced data review and “zero peak” work.

Or, if you prefer, switch to absolute minutes. Though keep in mind this setting is for **all** peaks in the quantitation method and cannot be changed on a compound by compound basis.

Properties Window



Right click **Properties** > **Fill Colors**.

Integrators

Choose the Right Integrator

Advanced Tasks

- Integration Parameters Setup
- Signal to Noise Setup
- Smoothing Setup

Mass Extraction Setup

- Spectrum Extraction Setup
- Isotopic Dilution Setup



| Sample | | | | | | |
|----------|--------------|------|-------|------------------|-------------------|--|
| Name | Data File | Type | Level | Acq. Method File | Acq. Date-Time | |
| Calib-L5 | CMAMCal_L5.d | Cal | L5 | APCIautotune.m | 5/12/2006 5:03 PM | |

| Quantifier | | | | | | | |
|------------|----|------|--------|-------|--------|--------------|--|
| Name | TS | Scan | Type | RT | Int. | Int. Params. | |
| Amp | 1 | MRM | Target | 2.102 | Agile2 | | |

| Qualifier | | | | |
|-----------|------------|-------------|--------------|--|
| MZ | Rel. Resp. | Uncertainty | Int. Params. | |
| 119.4 | 26.8 | 20.0 | | |



Integration

Integrator: **Agile2**

- Agile2
- Agile
- MS-MS
- MS-MS (GC)
- General
- Universal
- Spectrum Summation

Apply to All

OK Reset Default Cancel Apply

- **Method >Edit >Advanced Tasks > Integration Parameters Setup**
- Each compound can have its own integrator.
- Choose the one best suited for the compound's chromatography.
- Start with Agile2 (parameter-less) and move to other integrators if they work better.
- **All** integrators use Peak Filters.

Agile2

- 3rd generation parameter-less integrator
- Default Integrator
- Better baselines, higher sensitivity to smaller peaks

Agile

- 2nd generation parameter-less integrator

Universal

- 1st generation ChemStation integrator
- Familiar to GC LC ChemStation users

General (RTE)

- Familiar to MSD ChemStation users
- Areas in Universal are 10 time smaller than seen in ChemStation.

MS/MS and MS/MS (GC)

- 1st generation parameter-less integrator intended for MS/MS systems, not recommended for SQ. Originally required 64 data points.

ChemStation

- 2nd generation ChemStation
- Intended for UV

Integrators

General, Universal, Spectrum Summation

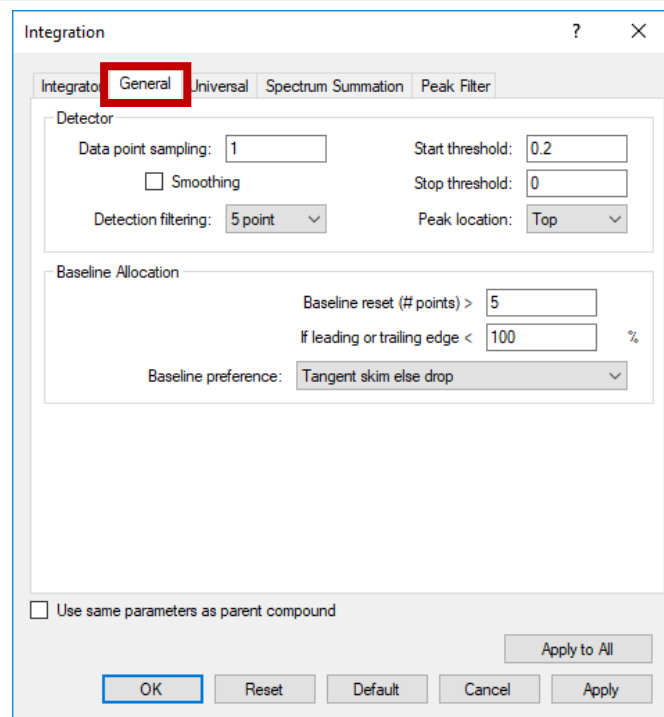
| Sample | | | | | |
|----------|--------------|------|-------|------------------|-------------------|
| Name | Data File | Type | Level | Acq. Method File | Acq. Date-Time |
| Calib-L5 | CMAMCal_L5.d | Cal | L5 | APC autotune.m | 5/12/2006 5:03 PM |

| Quantifier | | | | | | |
|------------|----|------|--------|-------|--------|------------|
| Name | TS | Scan | Type | RT | Int. | Int. Parm. |
| Amp | 1 | MRM | Target | 2.102 | Agile2 | |

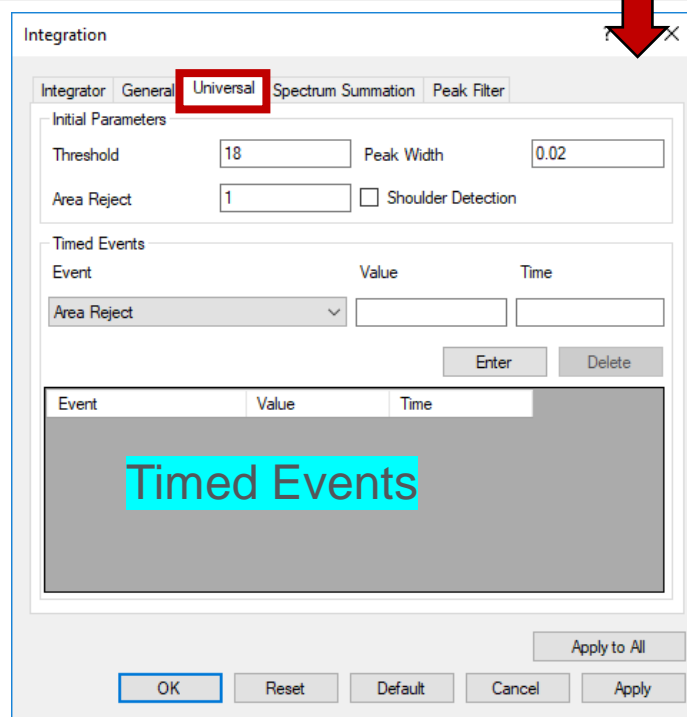
| Qualifier | | | |
|-----------|------------|-------------|------------|
| MZ | Rel. Resp. | Uncertainty | Int. Parm. |
| 119.4 | 26.8 | 20.0 | |

Adjust parameters as needed for each compound to get optimal integrations.

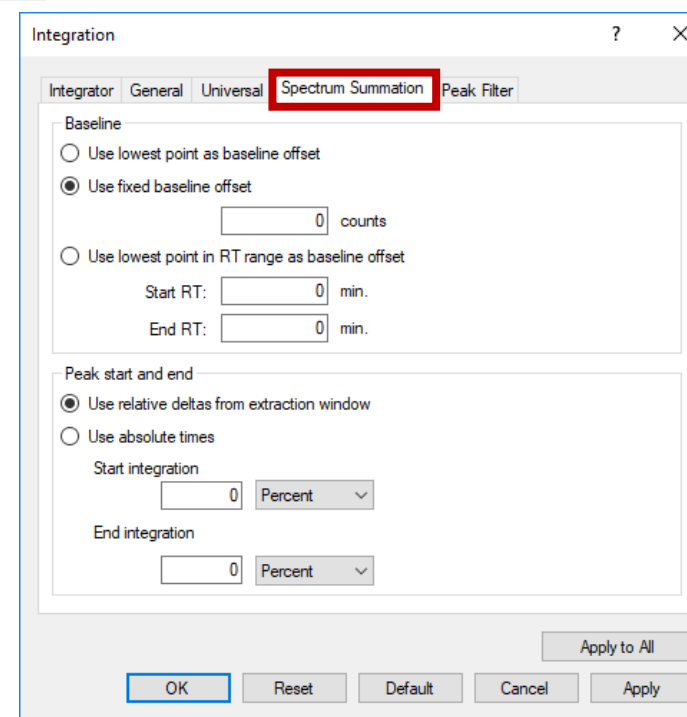
Tip: Evaluate low and high level calibrators.



Integration dialog box, General tab. The 'General' tab is selected and highlighted with a red box. Parameters include: Data point sampling: 1, Start threshold: 0.2, Stop threshold: 0, Detection filtering: 5 point, Peak location: Top, Baseline reset (# points) > 5, If leading or trailing edge < 100%, Baseline preference: Tangent skim else drop.



Integration dialog box, Universal tab. The 'Universal' tab is selected and highlighted with a red box. Parameters include: Threshold: 18, Peak Width: 0.02, Area Reject: 1, Shoulder Detection: unchecked. A table for Timed Events is visible with a red box around the text 'Timed Events'.



Integration dialog box, Spectrum Summation tab. The 'Spectrum Summation' tab is selected and highlighted with a red box. Parameters include: Baseline options (Use fixed baseline offset selected), Peak start and end options (Use relative deltas from extraction window selected).

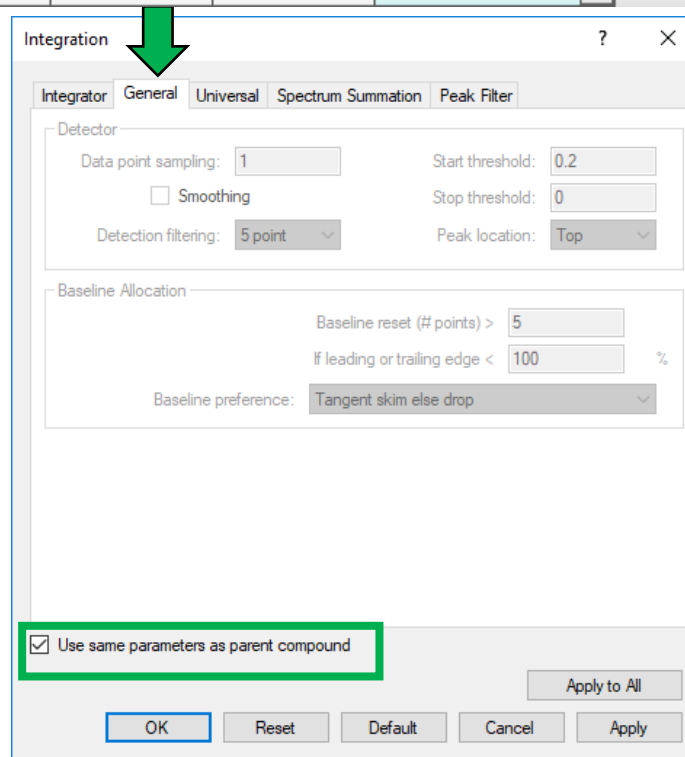
| Sample | | | | | | |
|----------|--------------|------|-------|------------------|-------------------|--|
| Name | Data File | Type | Level | Acq. Method File | Acq. Date-Time | |
| Calib-L5 | CMAMCal_L5.d | Cal | L5 | APClautotune.m | 5/12/2006 2:03... | |

| Qualifier | | | | | | | |
|-----------|----|---------------|------|--------|-------|---------|--------------|
| Name | TS | Transition | Scan | Type | RT | Int. | Int. Params. |
| Amp | 1 | 136.2 -> 91.4 | MRM | Target | 2.102 | General | ... |

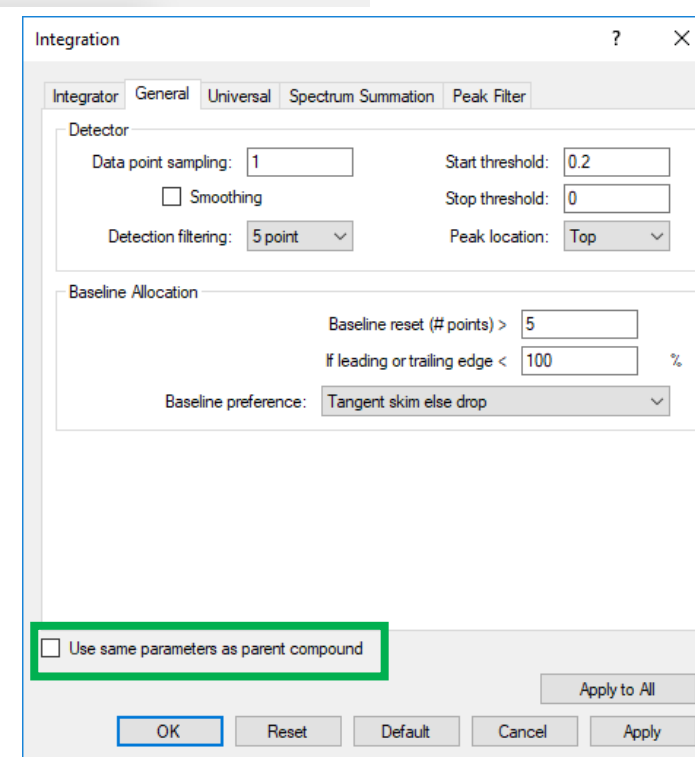
| Qualifier | | | | | | |
|---------------|-------------|----------------|------------|-------------|--------------|--|
| Precursor Ion | Product Ion | Transition | Rel. Resp. | Uncertainty | Int. Params. | |
| 136.2 | 119.4 | 136.2 -> 119.4 | 26.8 | 20.0 | | |

Qualifiers use the same integrator as quantifier.

If needed each qualifier may have separate parameters to optimize integration but the default is to use quantifier parameters.



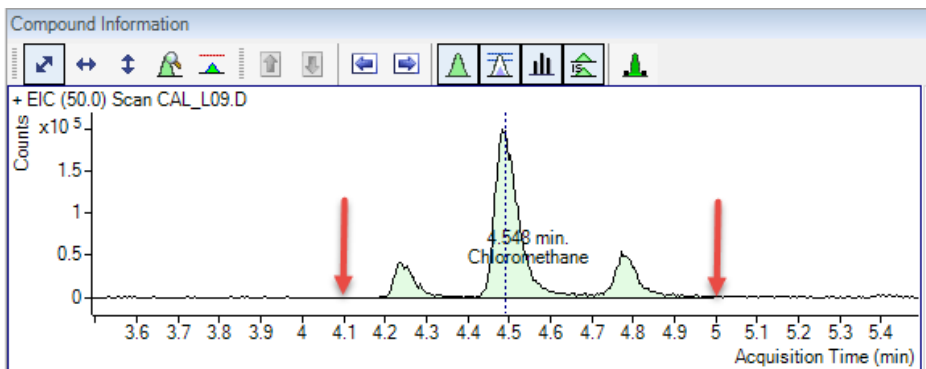
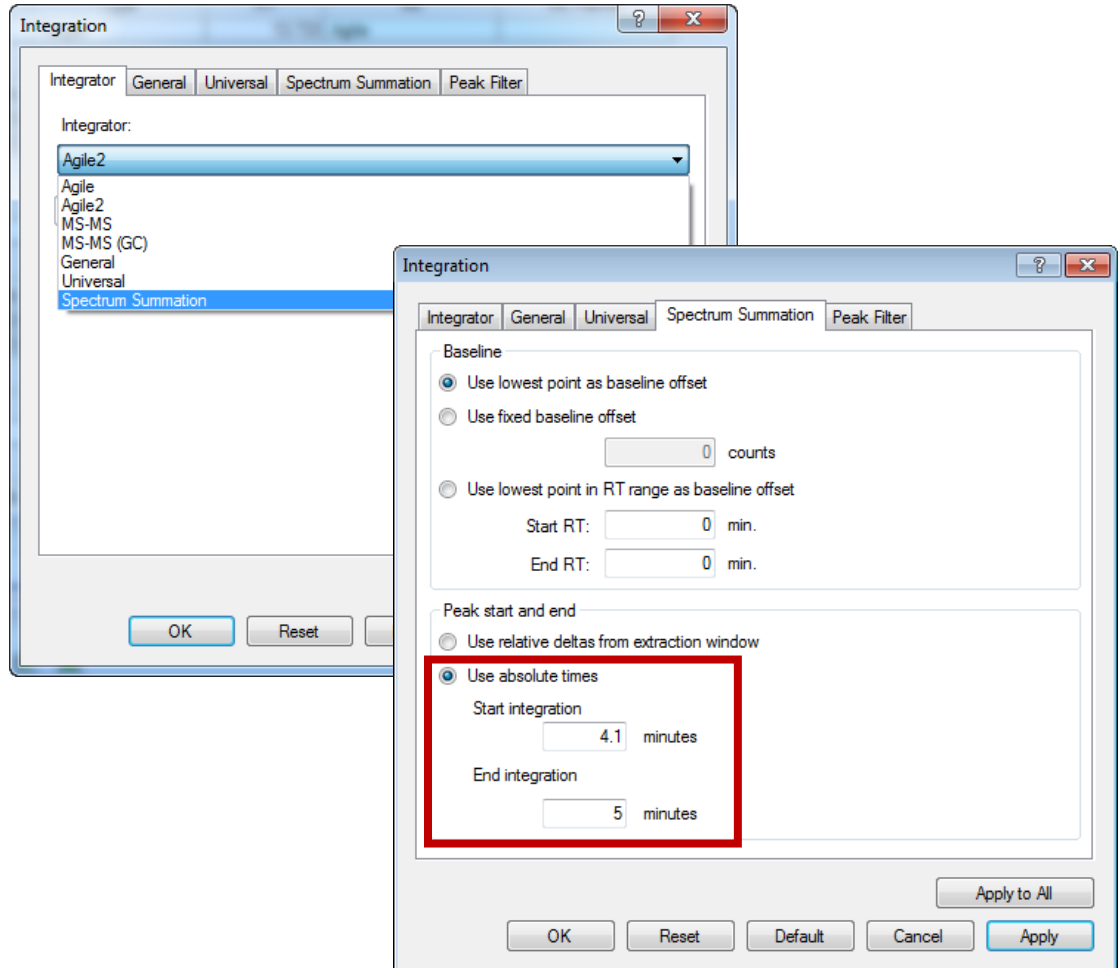
The Integration dialog box is shown with the 'General' tab selected. A green arrow points from the 'Int.' column of the Qualifier table to this dialog. At the bottom, the checkbox 'Use same parameters as parent compound' is checked and highlighted with a green box. Other settings include: Data point sampling: 1, Start threshold: 0.2, Stop threshold: 0, Smoothing: unchecked, Detection filtering: 5 point, Peak location: Top, Baseline reset (# points) >: 5, If leading or trailing edge <: 100 %, Baseline preference: Tangent skim else drop.



The Integration dialog box is shown with the 'General' tab selected. At the bottom, the checkbox 'Use same parameters as parent compound' is unchecked and highlighted with a green box. Other settings are identical to the first dialog: Data point sampling: 1, Start threshold: 0.2, Stop threshold: 0, Smoothing: unchecked, Detection filtering: 5 point, Peak location: Top, Baseline reset (# points) >: 5, If leading or trailing edge <: 100 %, Baseline preference: Tangent skim else drop.

Spectrum Summation Integrator

- Integrator designed for situations where compounds are poorly separated or peak shape is highly irregular such as
 - PCB mixtures
 - Fraction cut in hydrocarbons
 - Flow injection analysis (FIA)
- Sums signal over a time range.
- Exclude signal below threshold.
- Always gives a horizontal baseline.
- RT reported as the center of the time range.



Integrators

Peak Filters

- Available on all integrators including parameter-less ones.
- Separate Peak Filters for quantifier and qualifiers.
- Peak Filter is run after integrators create a peak list and then removes peak based on settings.
- Ideal to automatically remove small peaks that would otherwise require manual review and correction.

Default Setting for both Target and Qualifiers is Peak Area $\geq 5\%$ of largest peak.

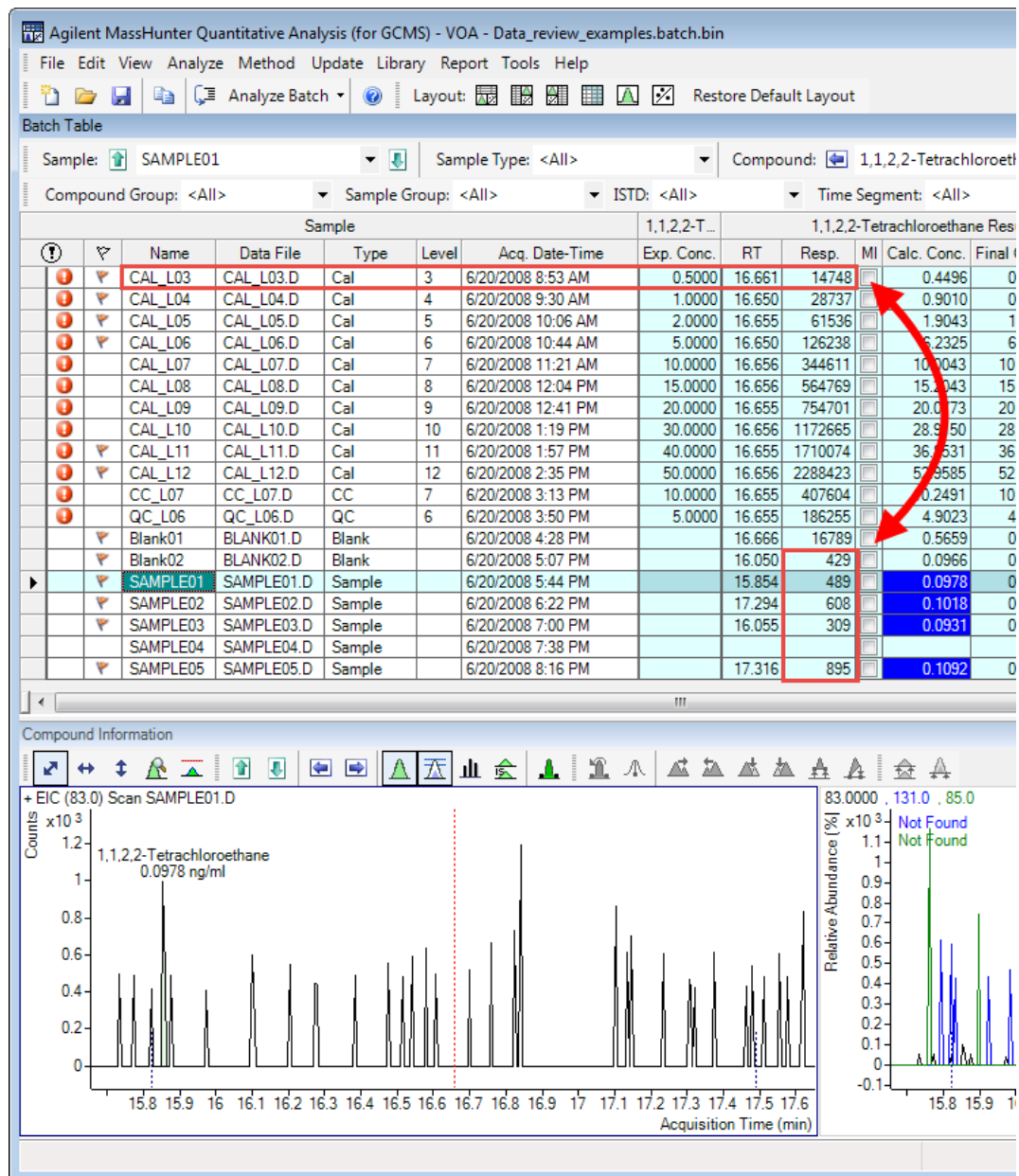
The screenshot shows the 'Integration' dialog box with the 'Peak Filter' tab selected. The 'Peak Threshold' section contains five radio button options: 'Peak Area (counts)' with a value of 10000, 'Peak Height (counts)' with a value of 10000, 'Peak Area (%)' with a value of 5 (selected), 'Peak Height (%)' with a value of 5, and 'Signal to Noise' with a value of 3. The 'Maximum number of peaks' section has a checkbox for 'Limit to the largest' which is unchecked, and a value of 100. At the bottom, there are buttons for 'OK', 'Reset', 'Default', 'Cancel', 'Apply', and 'Apply to All'.

Peak Filter Area

Typical noise or matrix peaks may be picked up by the integrator.

They are far too small relative to the response of the lowest level Calibrator to be reported. Normally we would need to “zero peak” each one.

Instead we can use peak filters in the method to remove the unwanted peaks.



Adjusting Peak Filter Area Thresholds Manual

Setting the peak area threshold for each compound would be a slow and tedious process...

The screenshot displays the Agilent MassHunter Quantitative Analysis interface. The main window shows a list of compounds in the Method Table:

| Name | TS | Scan | Type | RT | Int. | Int. Params. |
|---------------------------|------------|-------------|--------------|--------|-------|--------------|
| Styrene | 1 | Scan | Target | 16.544 | Agile | |
| Qualifier | | | | | | |
| MZ | Rel. Resp. | Uncertainty | Int. Params. | | | |
| 78.0 | 51.9 | 20.0 | | | | |
| 77.0 | 23.0 | 20.0 | | | | |
| 1,1,2,2-Tetrachloroethane | 1 | Scan | Target | 16.656 | Agile | |

The 'Integration' dialog box is open, showing the 'Peak Filter' tab. The 'Peak Threshold' section has the following settings:

- Peak Area (counts) >= 10000 counts
- Peak Height (counts) >= 10000 counts
- Peak Area (%) >= 5 % of largest peak
- Peak Height (%) >= 5 % of largest peak
- Signal to Noise >= 3

The 'Maximum number of peaks' section has the following settings:

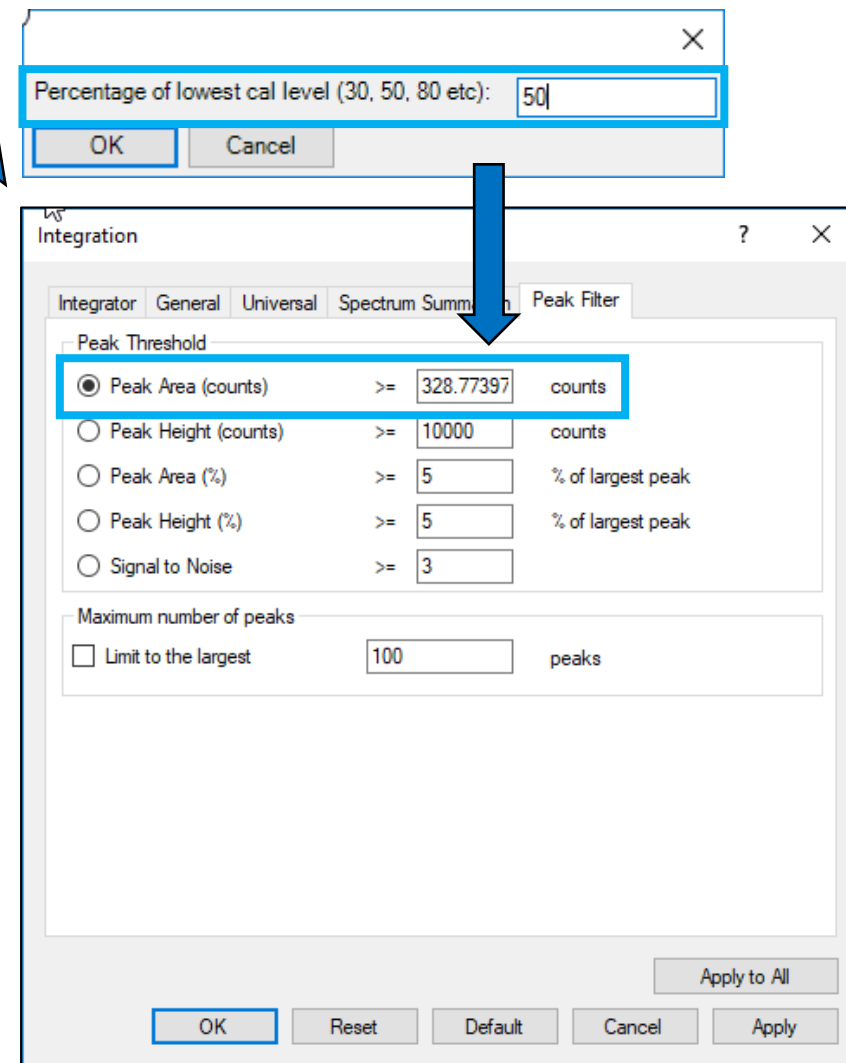
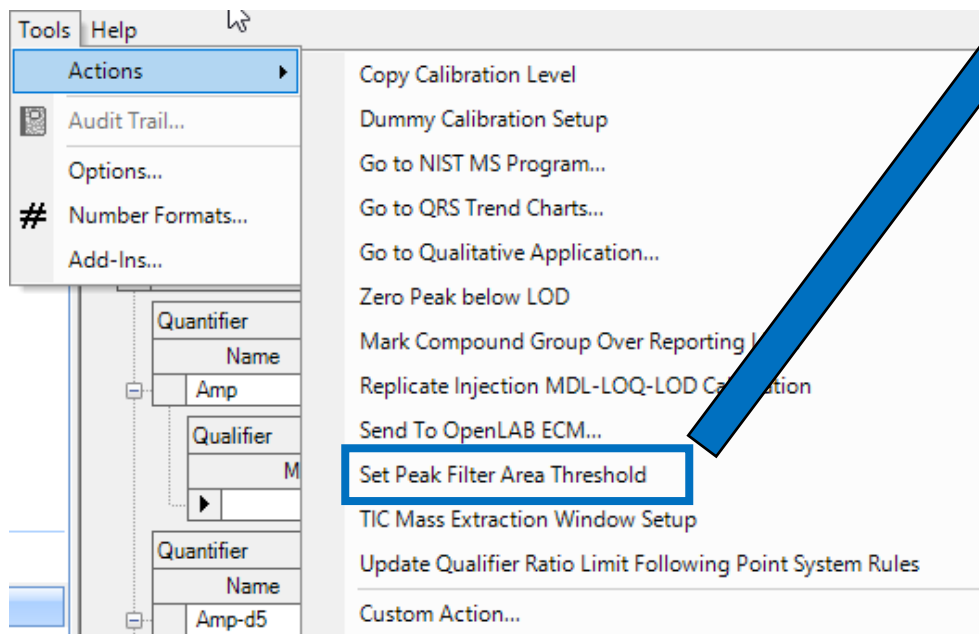
- Limit to the largest 100 peaks

The background shows a chromatogram with peaks for Styrene and 1,1,2,2-Tetrachloroethane. The x-axis is labeled 'Acquisition Time (min)' and the y-axis is labeled 'Counts x10³'.

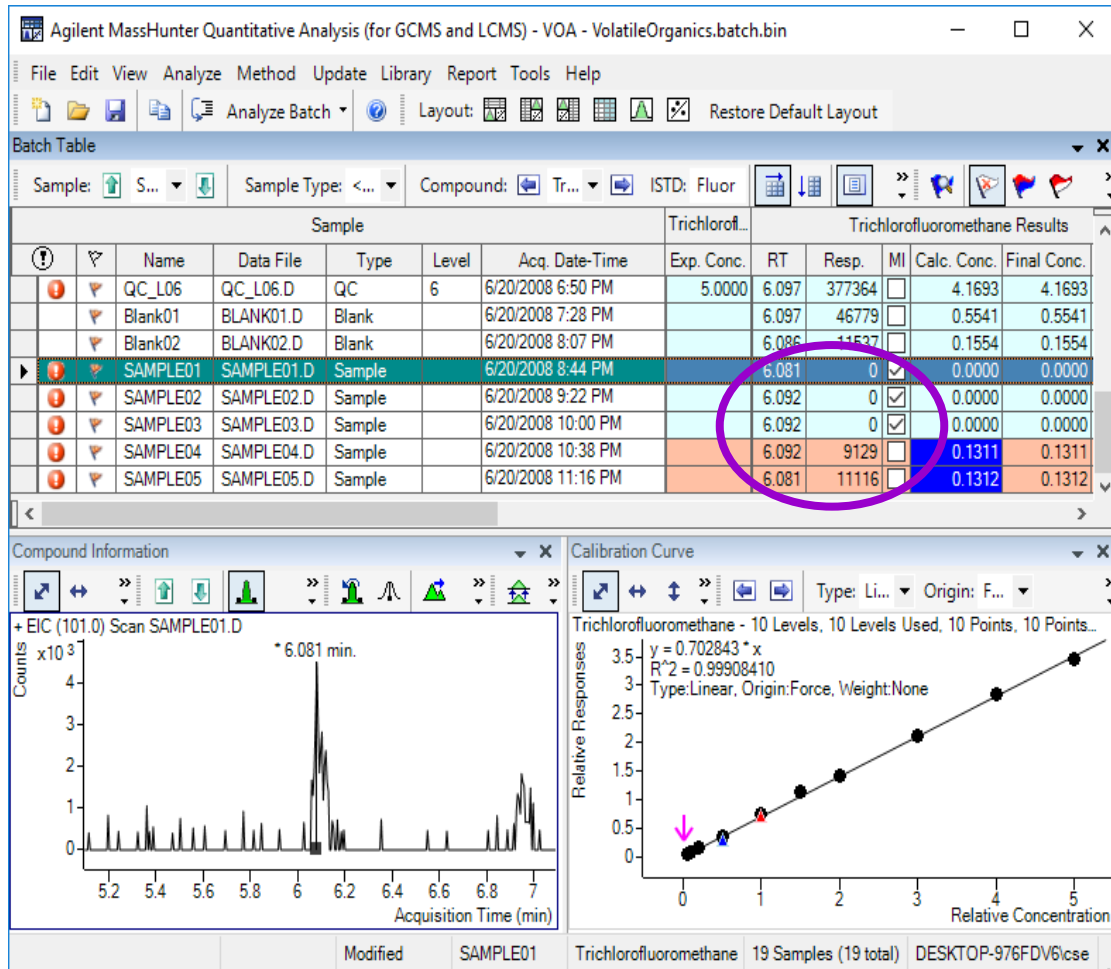
Adjusting Peak Filter Area Thresholds Automated

To automate the process, while in the Method Editor view, use the “Set Peak Filter Area Threshold” script to set each compound to a percent of its lowest Calibrator in the batch.

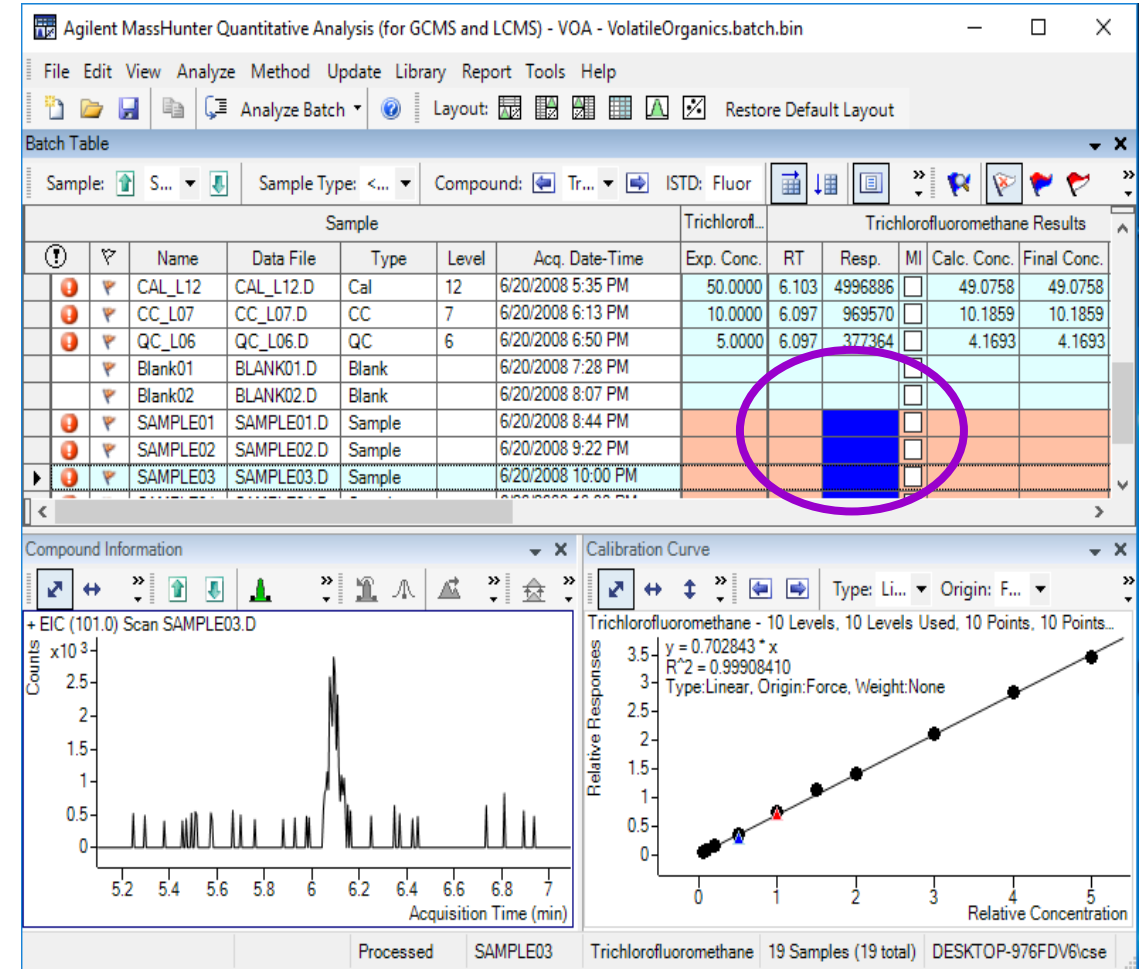
Tip: Establish calibration curve first.



Adjusting Peak Filter Area Thresholds Example



Before



After

Typical noise or matrix peaks are removed and require no data review or “zero peak” work.

Zero Peak Below LOD

| Sample | | | | | | 1,1,1-Tric... | 1,1,1-Trichloroethane Results | | | | | |
|--------|---|----------|------------|--------|-------|--------------------|-------------------------------|-------|--------|----|-------------|-------------|
| ? | ▼ | Name | Data File | Type | Level | Acq. Date-Time | Exp. Conc. | RT | Resp. | MI | Calc. Conc. | Final Conc. |
| ! | ▼ | CC_L07 | CC_L07.D | CC | 7 | 6/20/2008 6:13 PM | 10.0000 | 9.851 | 487439 | | 9.8663 | 9.8663 |
| ! | ▼ | QC_L06 | QC_L06.D | QC | 6 | 6/20/2008 6:50 PM | 5.0000 | 9.851 | 223375 | | 4.8593 | 4.8593 |
| | ▼ | Blank01 | BLANK01.D | Blank | | 6/20/2008 7:28 PM | | 9.862 | 19345 | | 0.6336 | 0.6336 |
| | ▼ | Blank02 | BLANK02.D | Blank | | 6/20/2008 8:07 PM | | 10.3 | 313 | | 0.2090 | 0.2090 |
| ▶ | ! | SAMPLE01 | SAMPLE01.D | Sample | | 6/20/2008 8:44 PM | | 10.1 | 305 | | 0.2081 | 0.2081 |
| ! | ▼ | SAMPLE02 | SAMPLE02.D | Sample | | 6/20/2008 9:22 PM | | 9.344 | 384 | | 0.2101 | 0.2101 |
| ! | ▼ | SAMPLE03 | SAMPLE03.D | Sample | | 6/20/2008 10:00 PM | | 9.949 | 485 | | 0.2136 | 0.2136 |
| ! | ▼ | SAMPLE04 | SAMPLE04.D | Sample | | 6/20/2008 10:38 P | | | | | | |

Method Editor > Outlier Setup Tasks > Limit of Detection.

- Eliminate peaks based on concentration rather than area.
- Must define the Limit of Detection outlier value for each compound.

Compound Information

+ EIC (99.0) Scan SAMPLE01.D

Counts x10³

10.173 min.

Acquisition Time (min)

Method Tasks

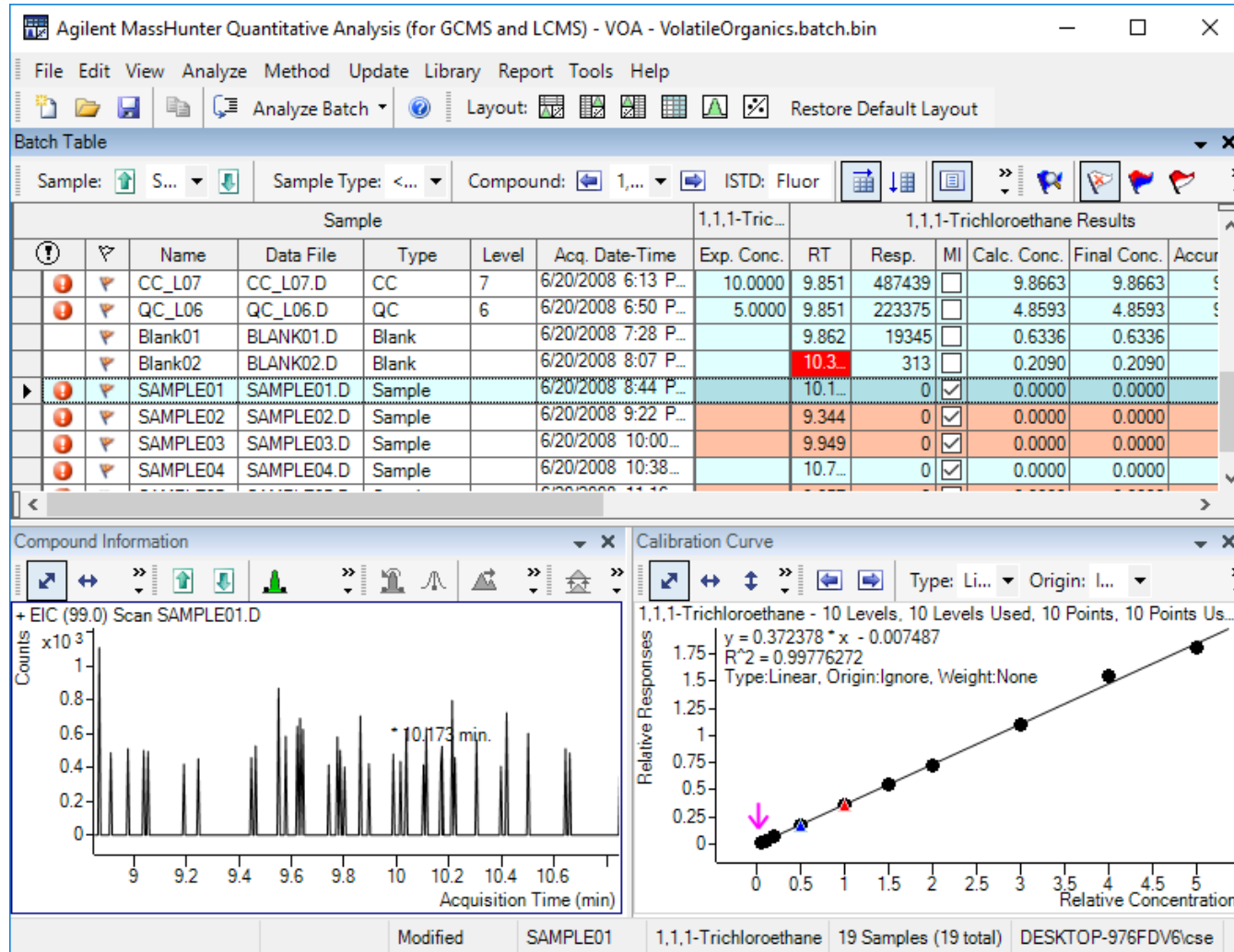
- Outlier Setup Tasks
- Retention Time
- Relative Retention...
- Peak Resolution
- Peak Symmetry
- Peak Full Width Hal...
- Peak Purity
- Plates
- Capacity Factor
- Signal-to-Noise Rat...
- Limit Of Detection

Method Table

| Sample | | | | | |
|----------|------------|--------|-------|------------------|----------|
| Name | Data File | Type | Level | Acq. Method File | Acq. Da |
| SAMPLE01 | SAMPLE01.D | Sample | | 624A.M | 6/20/200 |

| Quantifier | | | | |
|----------------------|----|------|--------|------|
| Name | TS | Scan | Type | LOD |
| 1,1,1-Trichloroet... | 1 | Scan | Target | 0.25 |
| 1,1,2,2-Tetrachl... | 1 | Scan | Target | 0.3 |
| 1,1,2-Trichloroet... | 1 | Scan | Target | 0.35 |
| 1,1-Dichloro-1-pr... | 1 | Scan | Target | 0.4 |
| 1,1-Dichloroetha... | 1 | Scan | Target | 0.45 |
| 1,1-Dichloroethe... | 1 | Scan | Target | 0.5 |
| 1,2,3-Trichlorob... | 1 | Scan | Target | 0.55 |

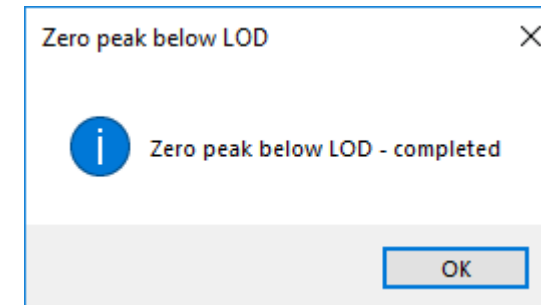
Zero Peak Below LOD



Tools > Actions > Zero Peak Below LOD

Tip: Review calibrators first.

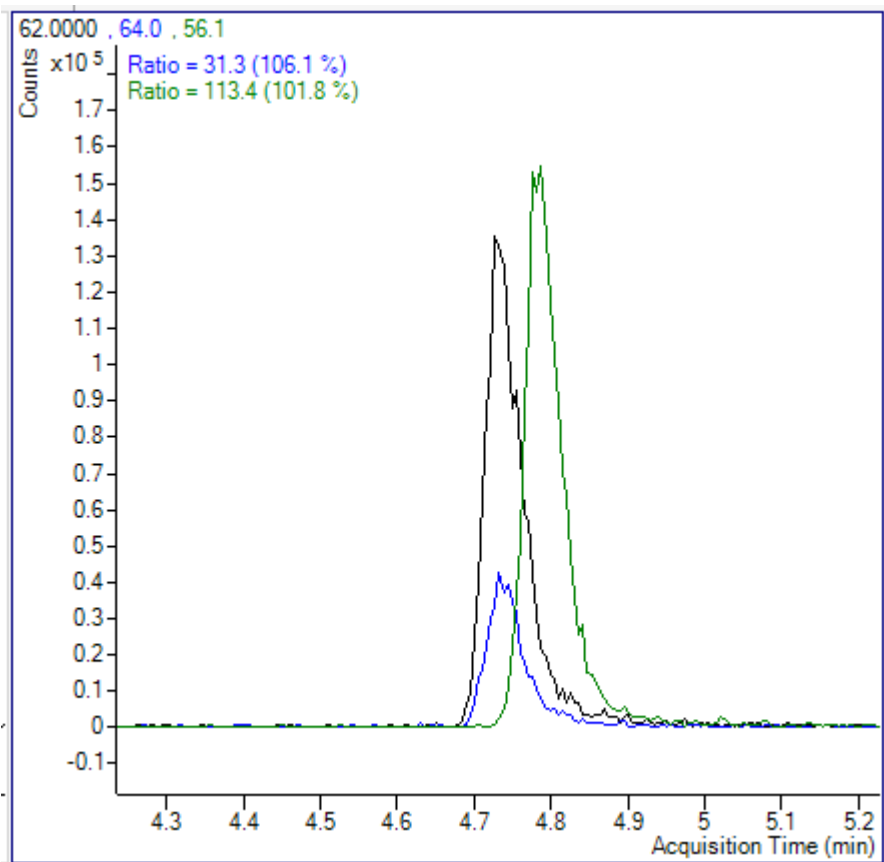
- Accessed from Batch Table View or Method Editor View.
- Zeros compounds if the Calculated Concentration is less than the LOD.



Correlation Window

The retention time difference limit of target ions to one or more qualifiers.

- Defines the maximum allowable variation of multiple extracted ion peak retention times before they are considered a single peak.
- Default time of 2.00 min is rather wide. Typically 0.01 to 0.05 min (0.6 sec to 3.0 sec).



Agilent MassHunter Quantitative Analysis (for GCMS) - Method - <C:\MassHunter\Data\QuantExamples\MS\VC>

File Edit View Analyze Method Update Library Report Tools Help

Analyze Batch Layout: Restore Default Layout

Method Tasks

- New / Open Method
- Workflow
- Method Setup Tasks
 - Compound Setup
 - Retention Time Setup
 - ISTD Setup
 - Concentration Setup
 - Qualifier Setup
 - Calibration Curve Setup
- Globals Setup
- Save / Exit
 - Validate
 - Save
 - Save As...
 - Exit

Method Table

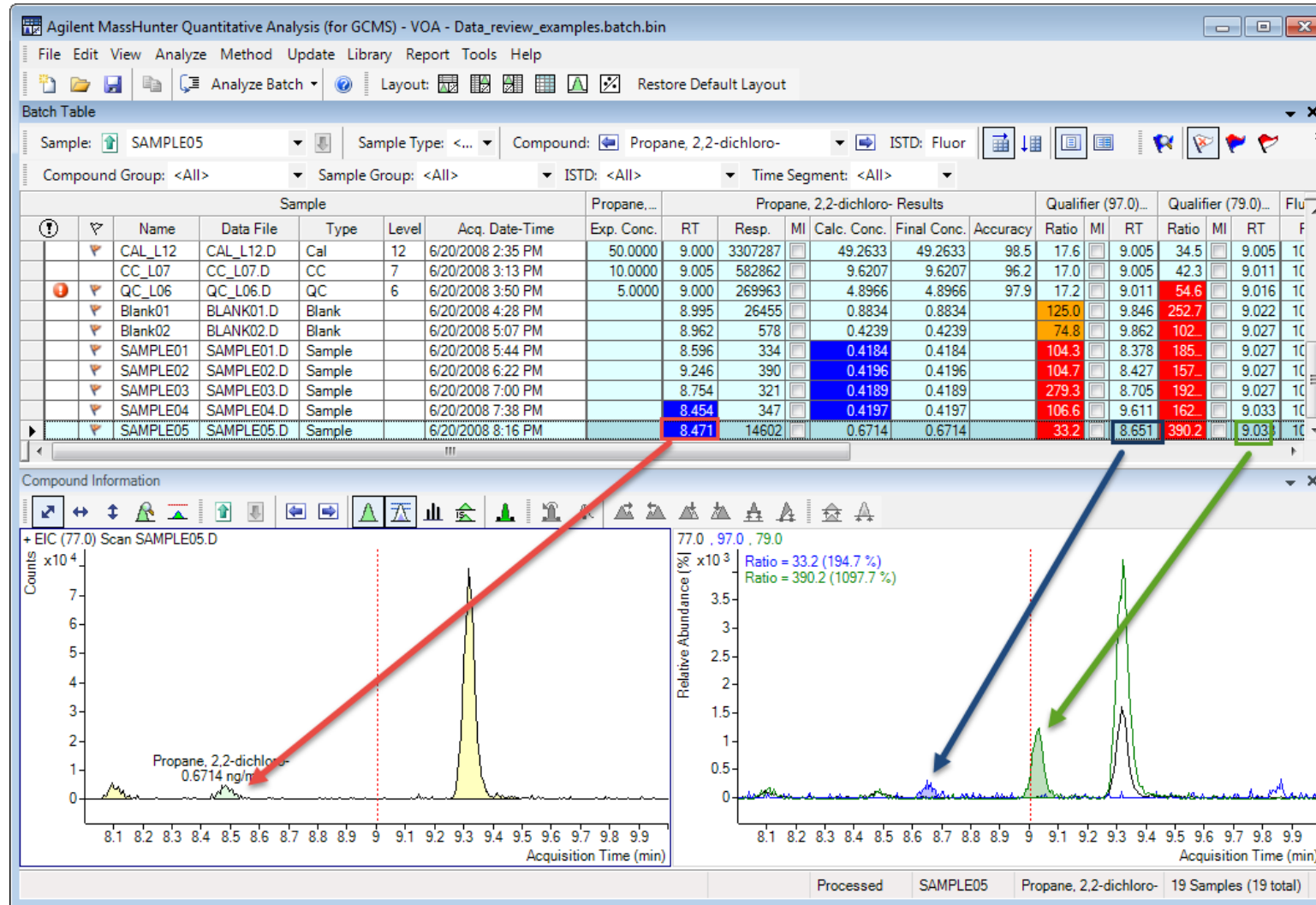
Time Segment: <All> Compound:

| Sample | | | |
|---------|-----------|------|-------|
| Name | Data File | Type | Level |
| CAL_L09 | CAL_L09.D | Cal | 9 |

Globals

| | |
|----------------------------------|-------------------------------------|
| Apply Multiplier to ISTD | <input type="checkbox"/> |
| Apply Multiplier to Matrix Spike | <input checked="" type="checkbox"/> |
| Apply Multiplier to Surrogate | <input checked="" type="checkbox"/> |
| Apply Multiplier to Target | <input checked="" type="checkbox"/> |
| Bracketing Type | None |
| CC Maximum Elapsed Time In Hours | 0.000 |
| Correlation Window | 2.000 |
| Dynamic Background Subtraction | <input type="checkbox"/> |
| Ignore Peaks Not Found | <input type="checkbox"/> |
| Library Method | / |
| Non Reference Window | 200.000 |
| Non Reference Window Type | Percent |
| Reference Library | C:\MassHunte...s.reflibrary.xml |

Correlation Window



Default value = 2.0 minutes.

Note that the retention times for target and qualifiers are different!

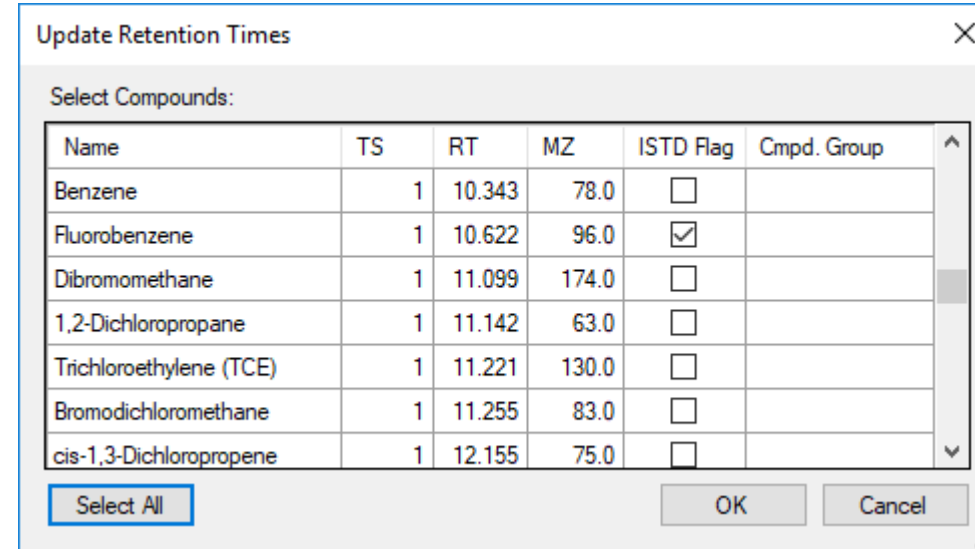
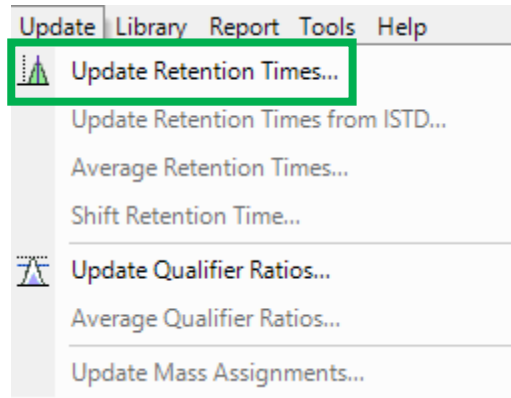
Retention times will Drift

- GC
 - Can use RTL locking to mitigate drift.
 - Use time reference compound in the middle of chromatographic run.
 - Make a single compound standard in the mid range of concentration.
 - Lock the method.
 - Relock the method as necessary.
- LC
 - Utilize a guard column.
 - Sample preparation steps.
 - Change solvents frequently to avoid microbial growth.
 - Clean solvent bottles when changing solvent.

But...retention times will still drift.

Retention Time Drift

Update Retention Times

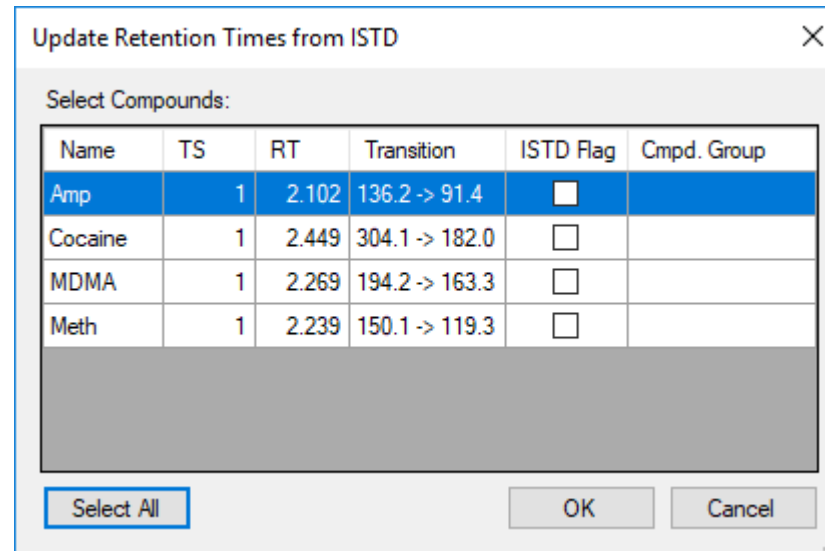
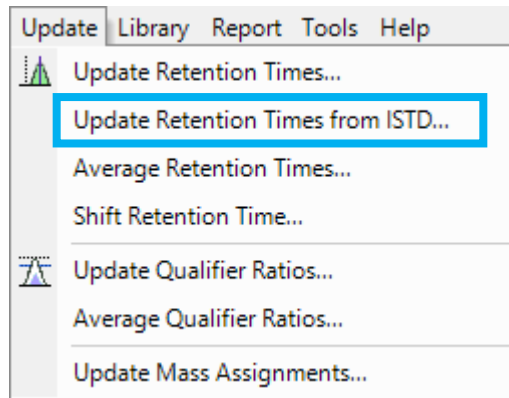


Update Retention Times is available in Batch Table View and Method Editor View.
Caveat - the compound must be found to update it.

Tip: Best updated from a mid range calibrator.

Retention Time Drift

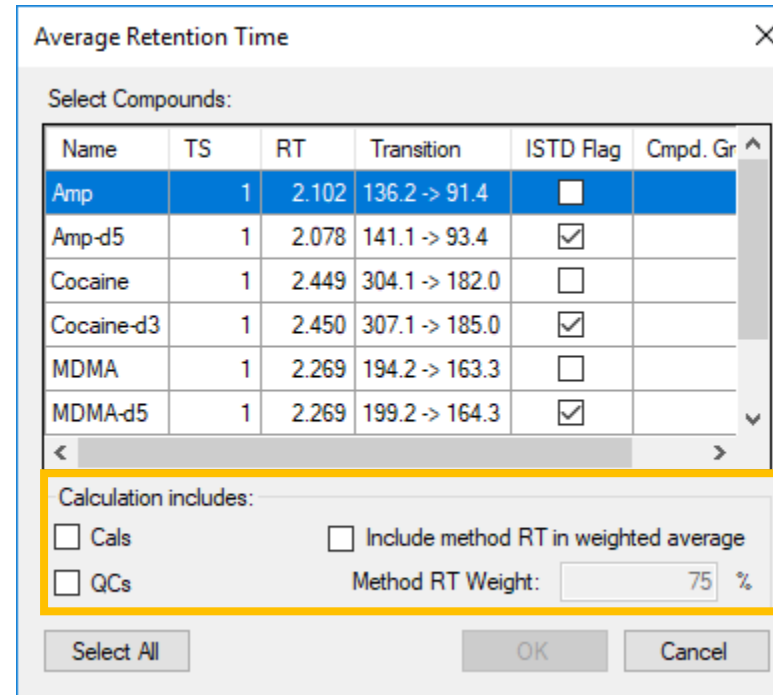
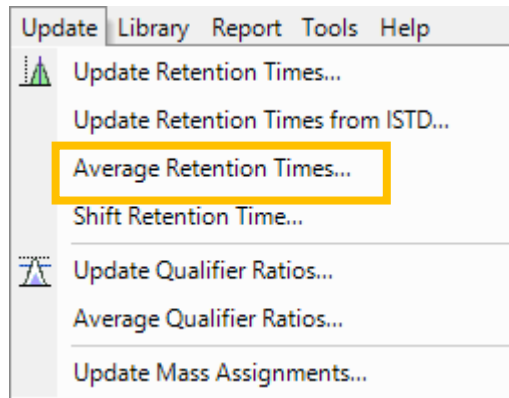
Update Retention Times from ISTD



- Update Retention Times from ISTD is a Method Editor feature.
- Particularly useful with isotopically labeled ISTD.
- **Tip: Remember Method Editor see one and only one sample—choose a calibrator.**

Retention Time Drift

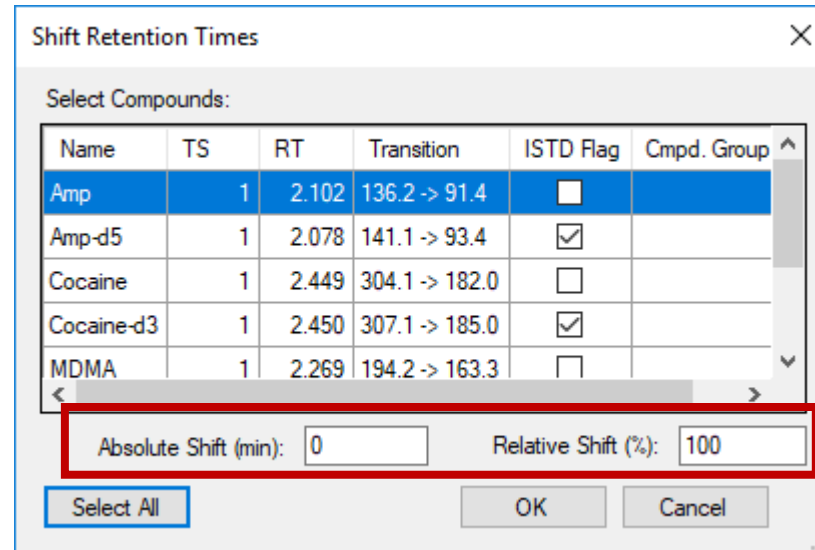
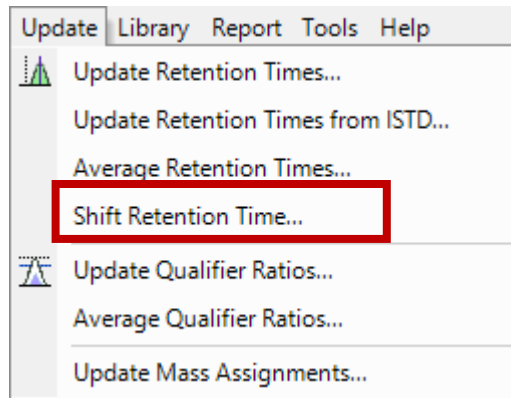
Average Retention Times



- Average Retention Times is a Method Editor feature.
- Allows choice of Cals or QCs or both.
- Includes a weighted average.

Retention Time Drift

Shift Retention Time



- Shift Retention Time is a Method Editor feature.
- Allows an Absolute Shift in minutes or a Relative Shift in percentage.
- Would be most applicable when changing columns.

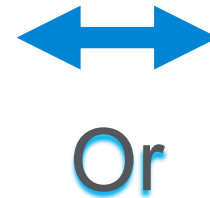
Qualifier Ion Ratios

Based on the sample currently loaded in Method Editor.

Tip: Choose a mid range calibrator before entering the Method Editor.

Update Qualifier Ratios

| Name | TS | RT | Transition | ISTD Flag | Cmpd. Gr |
|------------|----|-------|----------------|-------------------------------------|----------|
| Amp | 1 | 2.102 | 136.2 -> 91.4 | <input type="checkbox"/> | |
| Amp-d5 | 1 | 2.078 | 141.1 -> 93.4 | <input checked="" type="checkbox"/> | |
| Cocaine | 1 | 2.449 | 304.1 -> 182.0 | <input type="checkbox"/> | |
| Cocaine-d3 | 1 | 2.450 | 307.1 -> 185.0 | <input checked="" type="checkbox"/> | |
| MDMA | 1 | 2.269 | 194.2 -> 163.3 | <input type="checkbox"/> | |
| MDMA-d5 | 1 | 2.269 | 199.2 -> 164.3 | <input checked="" type="checkbox"/> | |



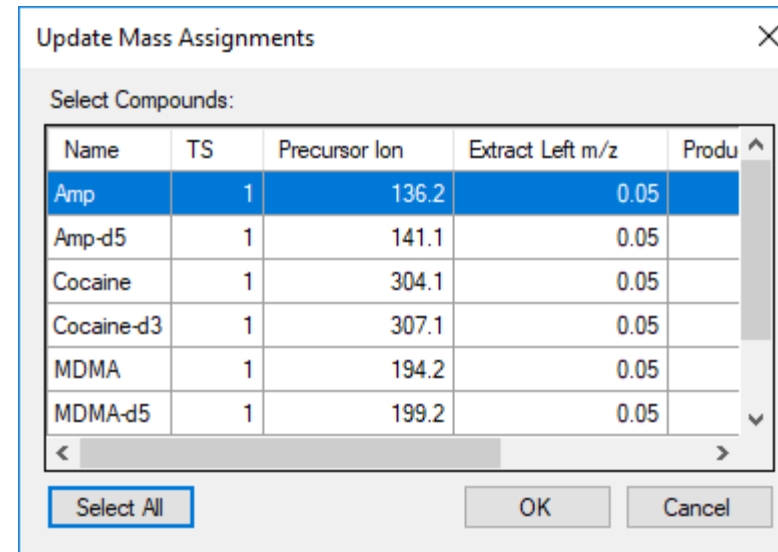
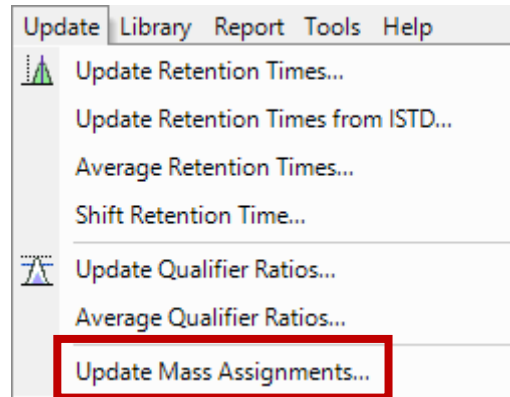
Average Qualifier Ratios

| Name | TS | RT | Transition | ISTD Flag | Cmpd. Gr |
|------------|----|-------|----------------|-------------------------------------|----------|
| Amp | 1 | 2.102 | 136.2 -> 91.4 | <input type="checkbox"/> | |
| Amp-d5 | 1 | 2.078 | 141.1 -> 93.4 | <input checked="" type="checkbox"/> | |
| Cocaine | 1 | 2.449 | 304.1 -> 182.0 | <input type="checkbox"/> | |
| Cocaine-d3 | 1 | 2.450 | 307.1 -> 185.0 | <input checked="" type="checkbox"/> | |
| MDMA | 1 | 2.269 | 194.2 -> 163.3 | <input type="checkbox"/> | |
| MDMA-d5 | 1 | 2.269 | 199.2 -> 164.3 | <input checked="" type="checkbox"/> | |
| Meth | 1 | 2.239 | 150.1 -> 119.3 | <input type="checkbox"/> | |
| Meth-d5 | 1 | 2.233 | 155.2 -> 92.3 | <input checked="" type="checkbox"/> | |

Calculation Includes:
 Cals
 QCs

Can use Cals and/or QCs.

Update Mass Assignments



- Update Mass Assignments is a Method Editor feature.
- It is based on currently selected sample in Batch Table.
- Useful with high resolution data (TOF and QTOF).

Reference Library

Globals Settings Option

- Activated from **Method > Edit > Library > Setup Reference Library**
- Reference Library may be obtained from a sample, preferably a calibrator, or from a small user generated library or a small subset library.
- Reference Library name is auto populated in Globals Settings.

Setup Reference Library

Obtain reference spectra from sample

Obtain reference spectra from lookup library

Lookup library:

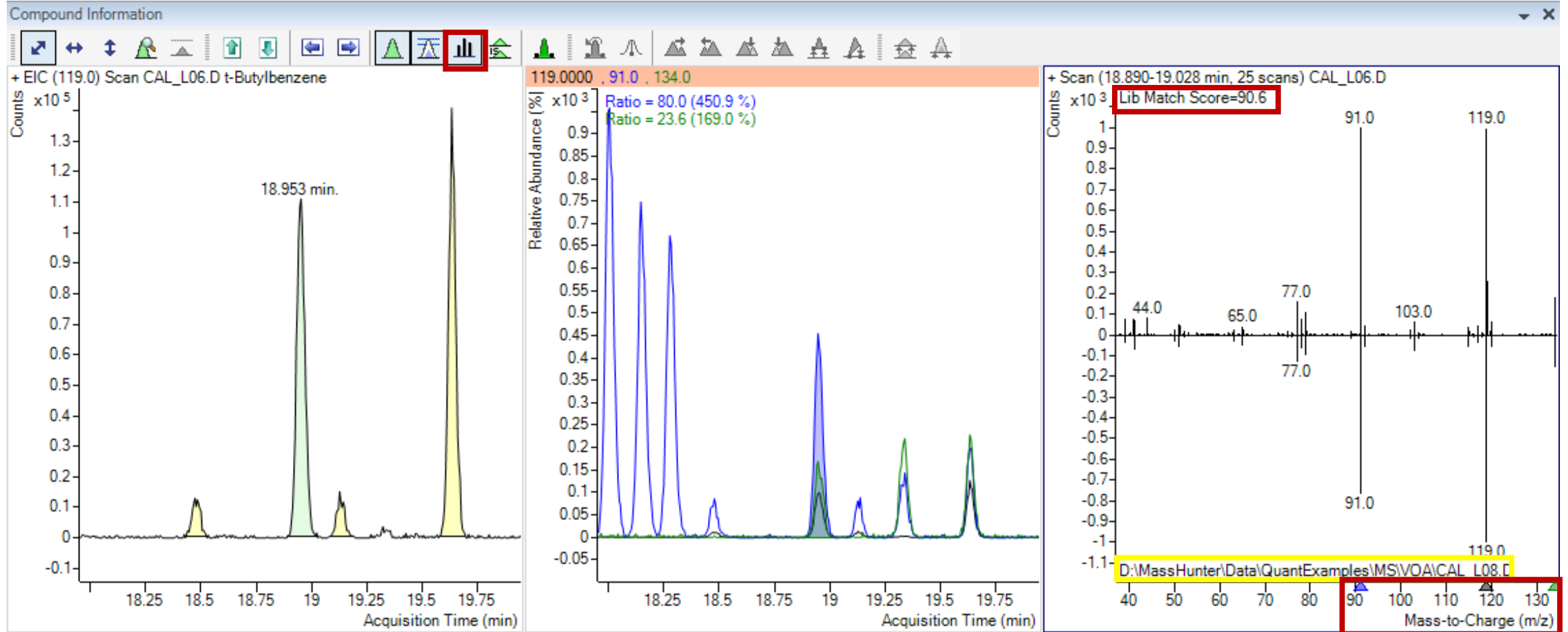
Create reference library at:

D:\MassHunter\Data\QuantExamples\MS\VOA\VolatileOrganics.reflibrary

OK Cancel

| Globals | |
|----------------------------------|---|
| Apply Multiplier to ISTD | <input type="checkbox"/> |
| Apply Multiplier to Matrix Spike | <input checked="" type="checkbox"/> |
| Apply Multiplier to Surrogate | <input checked="" type="checkbox"/> |
| Apply Multiplier to Target | <input checked="" type="checkbox"/> |
| Bracketing Type | None |
| Correlation Window | 2.000 |
| Dynamic Background Subtraction | <input type="checkbox"/> |
| Ignore Peaks Not Found | <input type="checkbox"/> |
| Library Method | |
| Non Reference Window | 200.000 |
| Non Reference Window Type | Percent |
| Reference Library | D:\MassHunter\Data\QuantE...VolatileOrganics.reflibrary.xml |
| Reference Pattern Library | |
| Reference Window | 80.000 |
| Reference Window Type | Percent |
| Relative ISTD | <input type="checkbox"/> |
| Standard Addition | <input type="checkbox"/> |

Reference Library Globals Settings Option



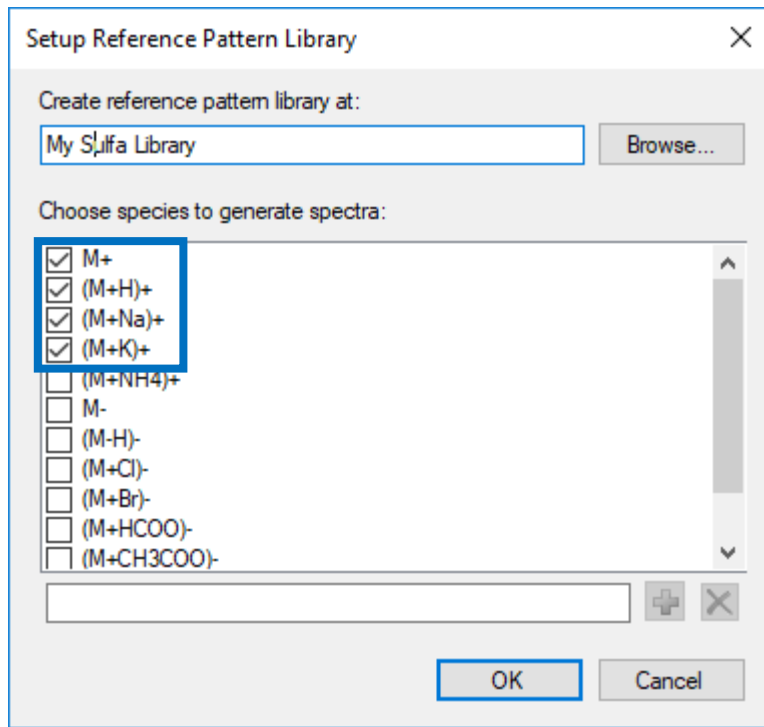
Appears in Compound Information window.

Customizable in **right click > Properties > Compound Information (2) tab.**

Reference Pattern Library

High Resolution Data

- Activated from **Method > Edit > Library > Setup Reference Pattern Library**.
- Can be obtained from a calibrator or from another library.
- Method must contain molecular formula.
- Reference Pattern Library name is populated in Globals.



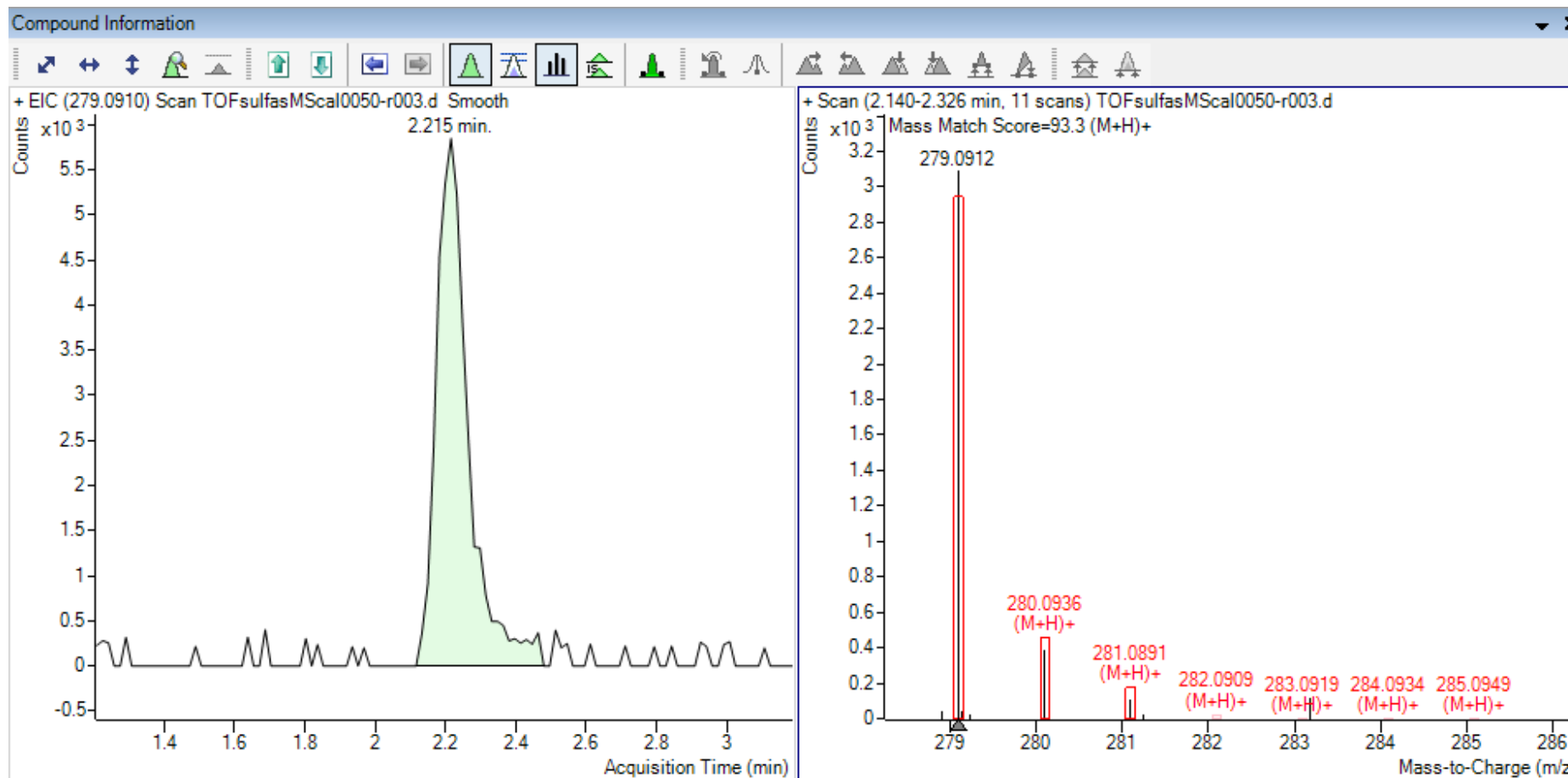
Select the adducts.

| Globals | |
|----------------------------------|-------------------------------------|
| Apply Multiplier to ISTD | <input type="checkbox"/> |
| Apply Multiplier to Matrix Spike | <input checked="" type="checkbox"/> |
| Apply Multiplier to Surrogate | <input checked="" type="checkbox"/> |
| Apply Multiplier to Target | <input checked="" type="checkbox"/> |
| Bracketing Type | None |
| Correlation Window | 2.000 |
| Ignore Peaks Not Found | <input type="checkbox"/> |
| Library Method | |
| Non Reference Window | 200.000 |
| Non Reference Window Type | Percent |
| Reference Library | |
| Reference Pattern Library | D:\MassHunter\...ern.reflibrary.xml |
| Reference Window | 80.000 |
| Reference Window Type | Percent |
| Relative ISTD | <input type="checkbox"/> |
| Standard Addition | <input type="checkbox"/> |
| SureMass | <input type="checkbox"/> |
| Use Profile Data | <input type="checkbox"/> |

Reference Pattern Library

High Resolution Data

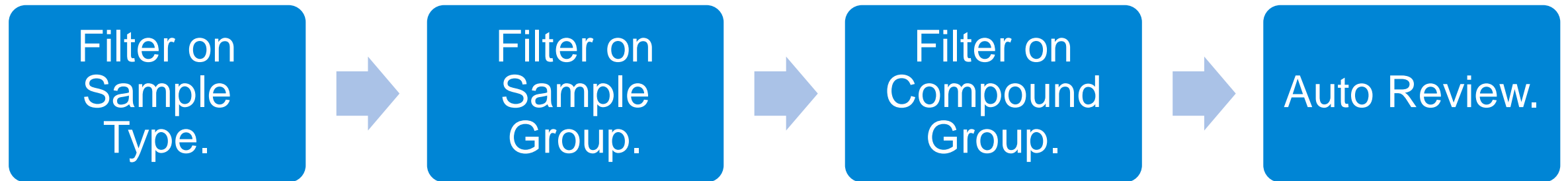
- Right click **Properties** > **Compound Information (2)** > **Reference pattern spectrum**
- Isotopic abundance and pattern appears in Spectrum window.





Demo time

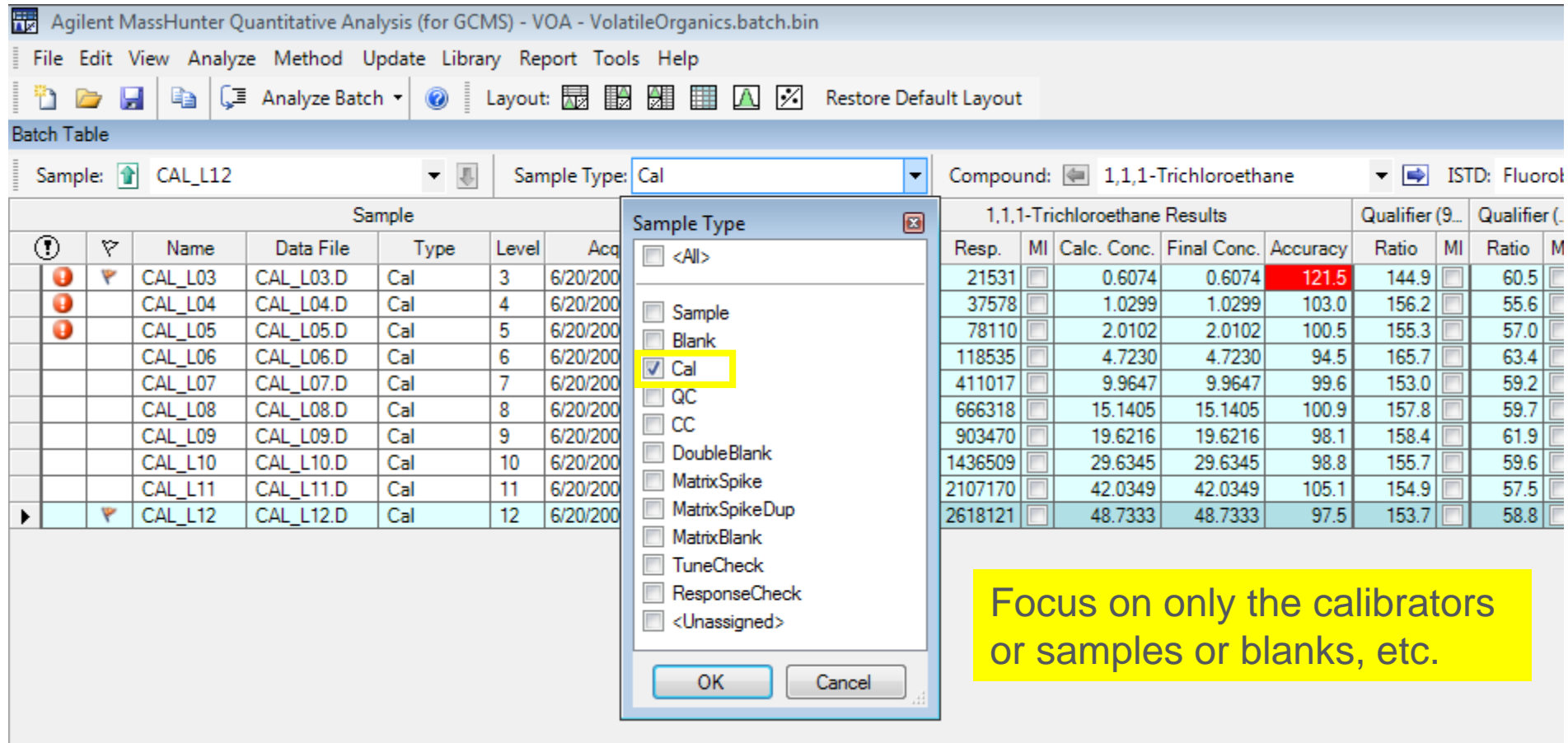
Data Review Check List



Data Review

Filter on Sample Type

Review Data in stages (Calibrators, then QC, then Samples).



Agilent MassHunter Quantitative Analysis (for GCMS) - VOA - VolatileOrganics.batch.bin

File Edit View Analyze Method Update Library Report Tools Help

Analyze Batch Layout: Restore Default Layout

Batch Table

Sample: CAL_L12 Sample Type: Cal Compound: 1,1,1-Trichloroethane ISTD: Fluorol

| Sample | | | | | | | 1,1,1-Trichloroethane Results | | | | Qualifier (9... | | Qualifier (. | | |
|--------|---------|-----------|------|-------|----------|--|-------------------------------|----|-------------|-------------|-----------------|-------|--------------|-------|---|
| | Name | Data File | Type | Level | Acq | | Resp. | MI | Calc. Conc. | Final Conc. | Accuracy | Ratio | MI | Ratio | M |
| ! | CAL_L03 | CAL_L03.D | Cal | 3 | 6/20/200 | | 21531 | | 0.6074 | 0.6074 | 121.5 | 144.9 | | 60.5 | |
| ! | CAL_L04 | CAL_L04.D | Cal | 4 | 6/20/200 | | 37578 | | 1.0299 | 1.0299 | 103.0 | 156.2 | | 55.6 | |
| ! | CAL_L05 | CAL_L05.D | Cal | 5 | 6/20/200 | | 78110 | | 2.0102 | 2.0102 | 100.5 | 155.3 | | 57.0 | |
| | CAL_L06 | CAL_L06.D | Cal | 6 | 6/20/200 | | 118535 | | 4.7230 | 4.7230 | 94.5 | 165.7 | | 63.4 | |
| | CAL_L07 | CAL_L07.D | Cal | 7 | 6/20/200 | | 411017 | | 9.9647 | 9.9647 | 99.6 | 153.0 | | 59.2 | |
| | CAL_L08 | CAL_L08.D | Cal | 8 | 6/20/200 | | 666318 | | 15.1405 | 15.1405 | 100.9 | 157.8 | | 59.7 | |
| | CAL_L09 | CAL_L09.D | Cal | 9 | 6/20/200 | | 903470 | | 19.6216 | 19.6216 | 98.1 | 158.4 | | 61.9 | |
| | CAL_L10 | CAL_L10.D | Cal | 10 | 6/20/200 | | 1436509 | | 29.6345 | 29.6345 | 98.8 | 155.7 | | 59.6 | |
| | CAL_L11 | CAL_L11.D | Cal | 11 | 6/20/200 | | 2107170 | | 42.0349 | 42.0349 | 105.1 | 154.9 | | 57.5 | |
| ▶ | CAL_L12 | CAL_L12.D | Cal | 12 | 6/20/200 | | 2618121 | | 48.7333 | 48.7333 | 97.5 | 153.7 | | 58.8 | |

Sample Type dialog box options:

- <All>
- Sample
- Blank
- Cal
- QC
- CC
- DoubleBlank
- MatrixSpike
- MatrixSpikeDup
- MatrixBlank
- TuneCheck
- ResponseCheck
- <Unassigned>

OK Cancel

Focus on only the calibrators or samples or blanks, etc.

Data Review

Sample Type

Sequence Table

New Sample(s) X [Download] [Download] Tools

| | Name | Vial | Method File | Data File | Type |
|---|------|------|-------------|---------------------|--------|
| 1 | Test | 1 | default.m | SequenceData-0001.d | Sample |

Sample
Blank
Cal
QC
Keyword
TuneCheck
MatrixBlank
MatrixSpike
MatrixSpikeDup
DoubleBlank
CC
ResponseCheck

- The Type or Sample Type is a parameter available in the sequence or worklist.
- Should be specified when data is acquired, but if necessary it can be entered in the Batch Table.
- In Sequence Table in GCMS software.
- In Worklist in LC MassHunter software.

Worklist

[New] [Refresh] [Print] [Run] [Pause] [Stop] [Help]

| | <input checked="" type="checkbox"/> | Sample Name | Sample Position | Method | Data File | Sample Type |
|---|-------------------------------------|-------------|-----------------|-----------|---------------------|-------------|
| 1 | <input checked="" type="checkbox"/> | Test | No Injection | default.m | WorklistData-0001.d | Sample |

Sample
Calibration
QC
Blank
DoubleBlank
Matrix
MatrixDup
MatrixBlank

Data Review

Filter on Sample Group

Sample Group is activated by right clicking on the toolbar.



Batch Table

Sample: QC-L4 Sample Type: <All> Compound: Amp

Compound Group: <All> Sample Group: <All> ISTD: <All> Time Segment: <All>

| Sample | | | | | | | |
|--------|---|----------|--------------|--------|-------|-------------------|--------------|
| | | Name | Data File | Type | Level | Acq. Date-Time | Sample Group |
| | ! | Blank-1 | CMAMBlk_01.d | Blank | | 5/12/2006 4:48 PM | Blank |
| | | Calib-L1 | CMAMCal_L1.d | Cal | L1 | 5/12/2006 4:51 PM | Cal |
| | | Calib-L2 | CMAMCal_L2.d | Cal | L2 | 5/12/2006 4:54 PM | Cal |
| | | Calib-L3 | CMAMCal_L3.d | Cal | L3 | 5/12/2006 4:57 PM | Cal |
| | | Calib-L4 | CMAMCal_L4.d | Cal | L4 | 5/12/2006 5:00 PM | Cal |
| | | Calib-L5 | CMAMCal_L5.d | Cal | L5 | 5/12/2006 5:03 PM | Cal |
| | | QC-L2 | CMAMQC_L2.d | QC | L2 | 5/12/2006 5:06 PM | QC |
| | | QC-L4 | CMAMQC_L4.d | QC | L4 | 5/12/2006 5:09 PM | QC |
| | ! | Sample-1 | CMAMSam_01.d | Sample | | 5/12/2006 5:12 PM | Sample Grp 1 |
| | | Sample-2 | CMAMSam_02.d | Sample | | 5/12/2006 5:15 PM | Sample Grp 2 |
| | | Sample-3 | CMAMSam_03.d | Sample | | 5/12/2006 5:18 PM | Sample Grp 1 |

Sample Group

- <All>
- Blank
- Cal
- QC
- Sample Grp 1
- Sample Grp 2

OK Cancel

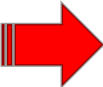
- This is helpful with large batches that contain several sample types.
- Sample Group is a column that can be added to the Worklist or Sequence Table.

Data Review

Filter on Compound Group

Compound groups are assigned in the Method Editor.

| Quantifier | | | | | | | | | |
|--------------------|----|------|--------|-------|--------|--------------|----------|-------------|---------------|
| Name | TS | Scan | Type | MZ | RT | Ion Polarity | Criteria | Cmpd. Group | Compound Math |
| 4,4'-Dibromooct... | 1 | Scan | ISTD | 456.0 | 12.808 | Positive | Close RT | | |
| Aldrin | 1 | Scan | Target | 263.0 | 19.671 | Positive | Close RT | | |
| Azinphos-ethyl | 1 | Scan | Target | 132.0 | 31.018 | Positive | Close RT | | |
| Azinphos-methyl | 1 | Scan | Target | 160.0 | 30.082 | Positive | Close RT | | |
| BHC alpha isom... | 1 | Scan | Target | 181.0 | 13.185 | Positive | Close RT | BHC | |
| BHC beta isomer | 1 | Scan | Target | 219.0 | 14.327 | Positive | Close RT | BHC | |
| BHC delta isomer | 1 | Scan | Target | 181.0 | 15.693 | Positive | Close RT | BHC | |
| BHC Total | 1 | Scan | Target | 100.0 | 15.000 | Positive | Close RT | BHC | |
| Carbophenothion | 1 | Scan | Target | 157.0 | 27.267 | Positive | Close RT | | |
| Chlorpyrifos | 1 | Scan | Target | 197.0 | 20.355 | Positive | Close RT | | |



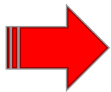
Response Sum
Response Average
Concentration Sum
Concentration Average
TPH Subtraction

- Compound groups are useful for parent compound and metabolites.
- Reviewing Aroclor congeners by group (PCB).

Data Review

Filter on Compound Group

Compounds may be assigned to more than one group by separating the group names using commas.



Agilent MassHunter Quantitative Analysis (for GCMS) - Method - <C:\MassHunter\Data\QuantExamples\MS\VOA\QuantResults\Data_review_examples.batch.bi

File Edit View Analyze Method Update Library Report Tools Help

Analyze Batch Layout: Restore Default Layout

Method Tasks: New / Open Method Workflow Method Setup Tasks

Compound Setup Retention Time Setup ISTD Setup Concentration Setup Qualifier Setup

Time Segment: <All> Compound: t-butyl Acetate Reset Table View

| Quantifier | Name | TS | Scan | Type | MZ | RT | Ion Polarity | Criteria | Cmpd. Group |
|------------|------------------------|----|------|-----------|-------|--------|--------------|----------|-------------|
| | 1,2-Dichloroethane-d4 | 1 | Scan | Surrogate | 65.0 | 9.595 | Positive | Close RT | Surrogate |
| | 1,2-Dichloroethane | 1 | Scan | Target | 62.0 | 9.696 | Positive | Close RT | Pest |
| | 1,1,1-Trichloroethane | 1 | Scan | Target | 99.0 | 9.850 | Positive | Close RT | Pest |
| | 1,1-Dichloro-1-propene | 1 | Scan | Target | 75.0 | 10.100 | Positive | Close RT | Herb |
| | Carbon Tetrachloride | 1 | Scan | Target | 117.0 | 10.328 | Positive | Close RT | Pest |
| | Benzene | 1 | Scan | Target | 78.0 | 10.343 | Positive | Close RT | Pest |
| | Fluorobenzene | 1 | Scan | ISTD | 96.0 | 10.622 | Positive | Close RT | ISTD |

Review Compounds by Group (using Compound Table View).

Agilent MassHunter Quantitative Analysis (for GCMS) - VOA - Data_review_examples.batch.bin

File Edit View Analyze Method Update Library Report Tools Help

Analyze Batch Layout: Restore Default Layout

Batch Table

Sample: CAL_L04 Sample Type: <All> Compound: 1,1,1-Trichloroethane ISTD: Fluorobenzene

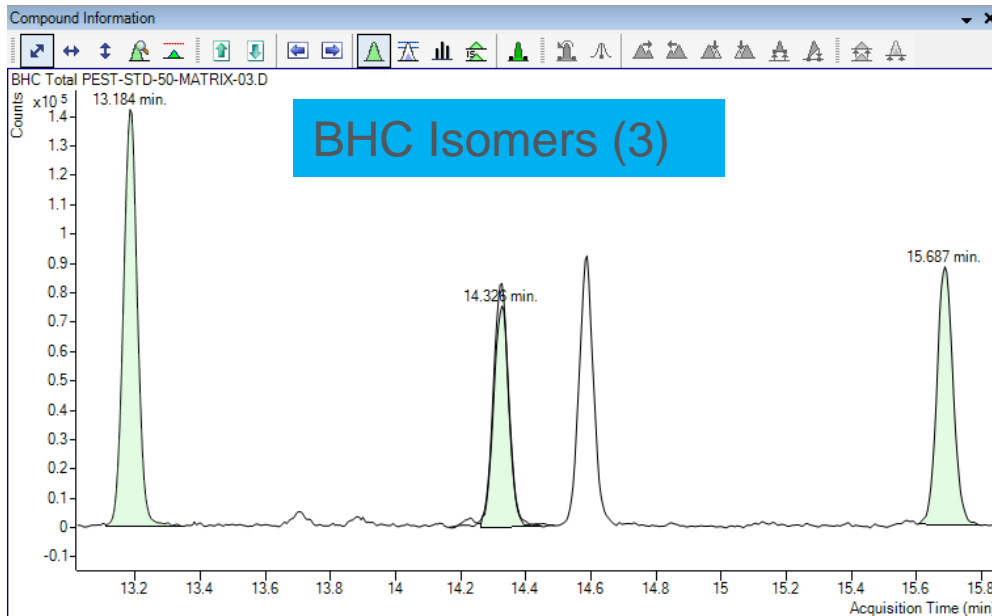
Compound Group: Pest Sample Group: <All> ISTD: <All> Time Segment: <All>

| Co | Herb | ISTD | CAL_L04 | | | | | | Qualifier 1. | | Qualifier 2. | | ISTD Method | | ISTD Results | | ISTD Qual. | | ISTD Qual. | |
|----|------|-----------|---------|-------|----|-------------|-------------|----------|--------------|----|--------------|----|------------------------|--------|--------------|-------|------------|-------|------------|--|
| | | | RT | Resp. | MI | Calc. Conc. | Final Conc. | Accuracy | Ratio | MI | Ratio | MI | Name | RT | Resp. | Ratio | MI | Ratio | MI | |
| | | Pest | | | | | | 61.3 | 30.2 | | | | Fluorobenzene | 10.621 | 1183924 | 1.8 | | 10.1 | | |
| | | Surrogate | 4.493 | 42888 | | 1.1095 | 1.1095 | 110.9 | 20.5 | | | | Fluorobenzene | 10.621 | 1183924 | 1.8 | | 10.1 | | |
| | | <All> | 19.542 | 78242 | | 1.0327 | 1.0327 | 103.3 | 62.4 | | 46.5 | | 1,4-Dichlorobenzene-d4 | 19.493 | 583143 | 57.3 | | 40.9 | | |
| | | | 4.728 | 46684 | | 0.6708 | 0.6708 | 67.1 | 21.4 | | | | Fluorobenzene | 10.621 | 1183924 | 1.8 | | 10.1 | | |
| | | | 23.290 | 45377 | | 1.4642 | 1.4642 | 146.4 | 94.7 | | 32.1 | | 1,4-Dichlorobenzene-d4 | 19.493 | 583143 | 57.3 | | 40.9 | | |
| | | | 5.235 | 25606 | | 1.3296 | 1.3296 | 133.0 | 78.7 | | | | Fluorobenzene | 10.621 | 1183924 | 1.8 | | 10.1 | | |
| | | | 5.404 | 20635 | | 0.9149 | 0.9149 | 91.5 | 37.7 | | | | Fluorobenzene | 10.621 | 1183924 | 1.8 | | 10.1 | | |
| | | | 23.678 | 63270 | | 1.3015 | 1.3015 | 130.2 | 10.4 | | 11.9 | | 1,4-Dichlorobenzene-d4 | 19.493 | 583143 | 57.3 | | 40.9 | | |
| | | | 23.852 | 12285 | | 0.8284 | 0.8284 | 82.8 | | | | | 1,4-Dichlorobenzene-d4 | 19.493 | 583143 | 57.3 | | 40.9 | | |
| | | | 6.092 | 90617 | | 0.7192 | 0.7192 | 71.9 | 64.1 | | 3.9 | | Fluorobenzene | 10.621 | 1183924 | 1.8 | | 10.1 | | |
| | | | 6.185 | 29268 | | 0.6327 | 0.6327 | 63.3 | 37.6 | | | | Fluorobenzene | 10.621 | 1183924 | 1.8 | | 10.1 | | |

Data Review

Compound Information

Compound groups are shown in the Compound information window.

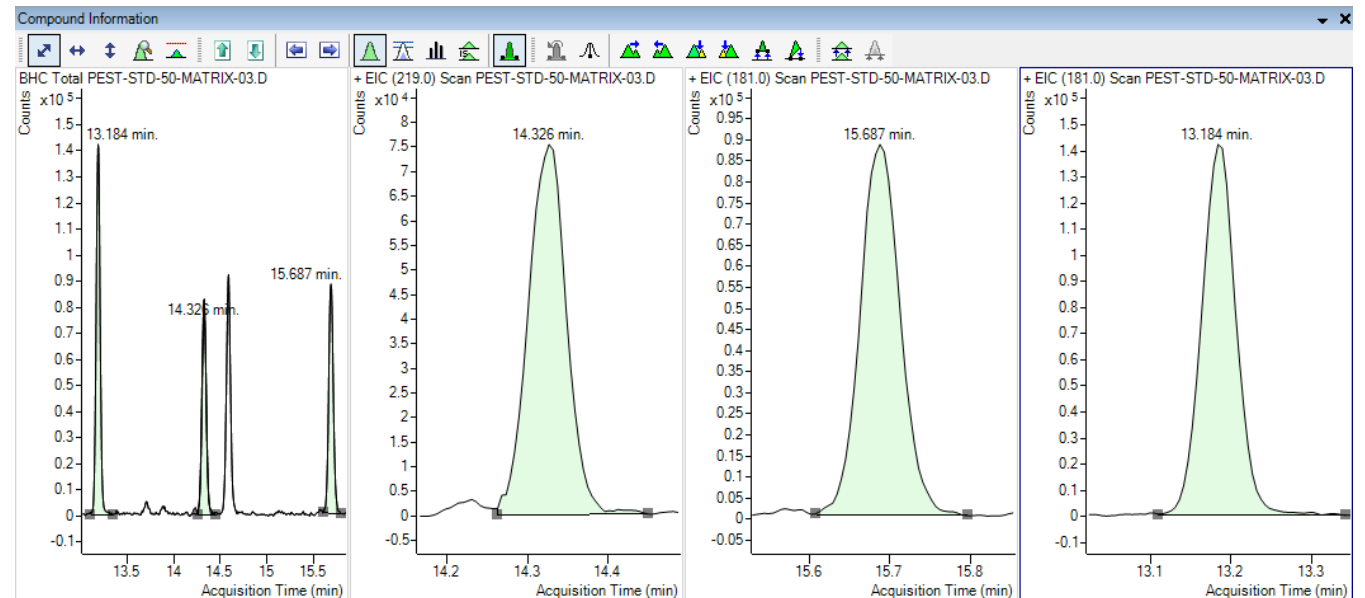


Tip: Right click Properties > Compound Information (2) Manual integration > Max # panes per row.

Manual integration: _____

Show baseline start/end boxes

Max. # of panes per row:

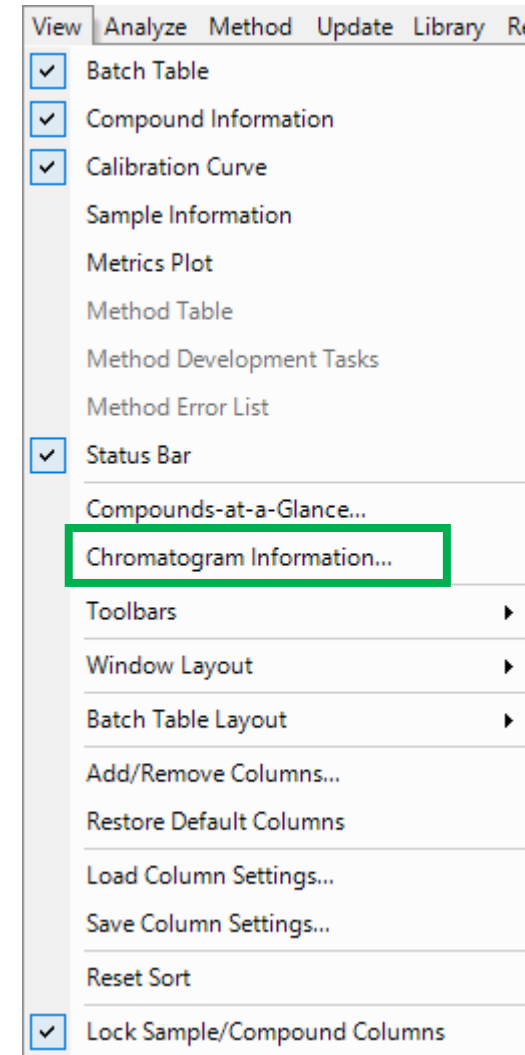
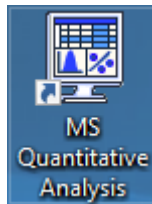
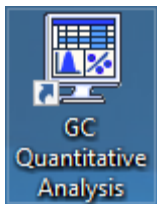


Manual Integration turned on.

Data Review

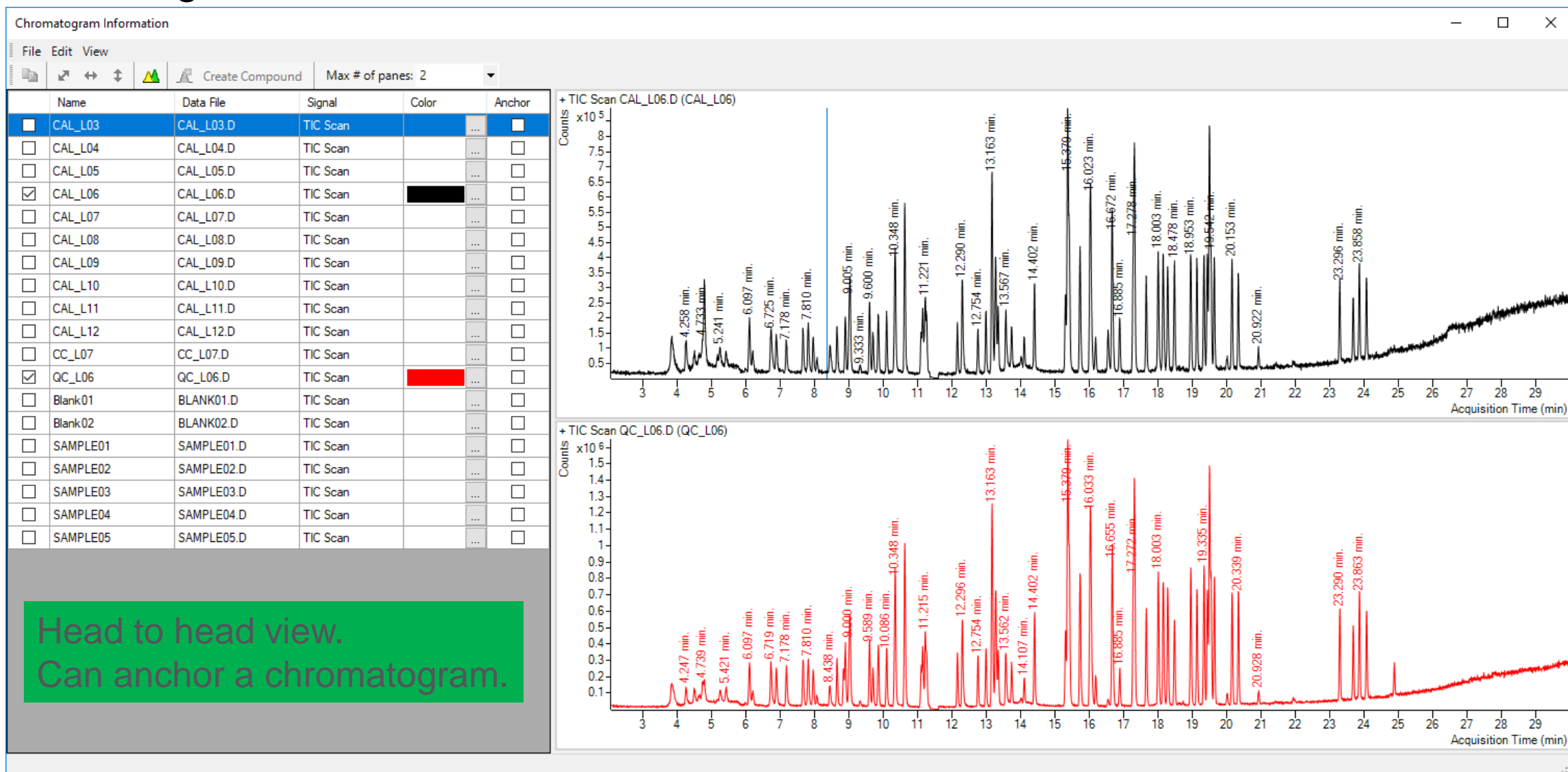
Chromatogram Information

- Accessed from **View > Chromatogram Information**.
- Useful to compare multiple chromatograms.
- Useful to compare patterns.
- Create Compounds GC Data only → Method Editor.
- Available for GC and MS Quantitative Analysis only.



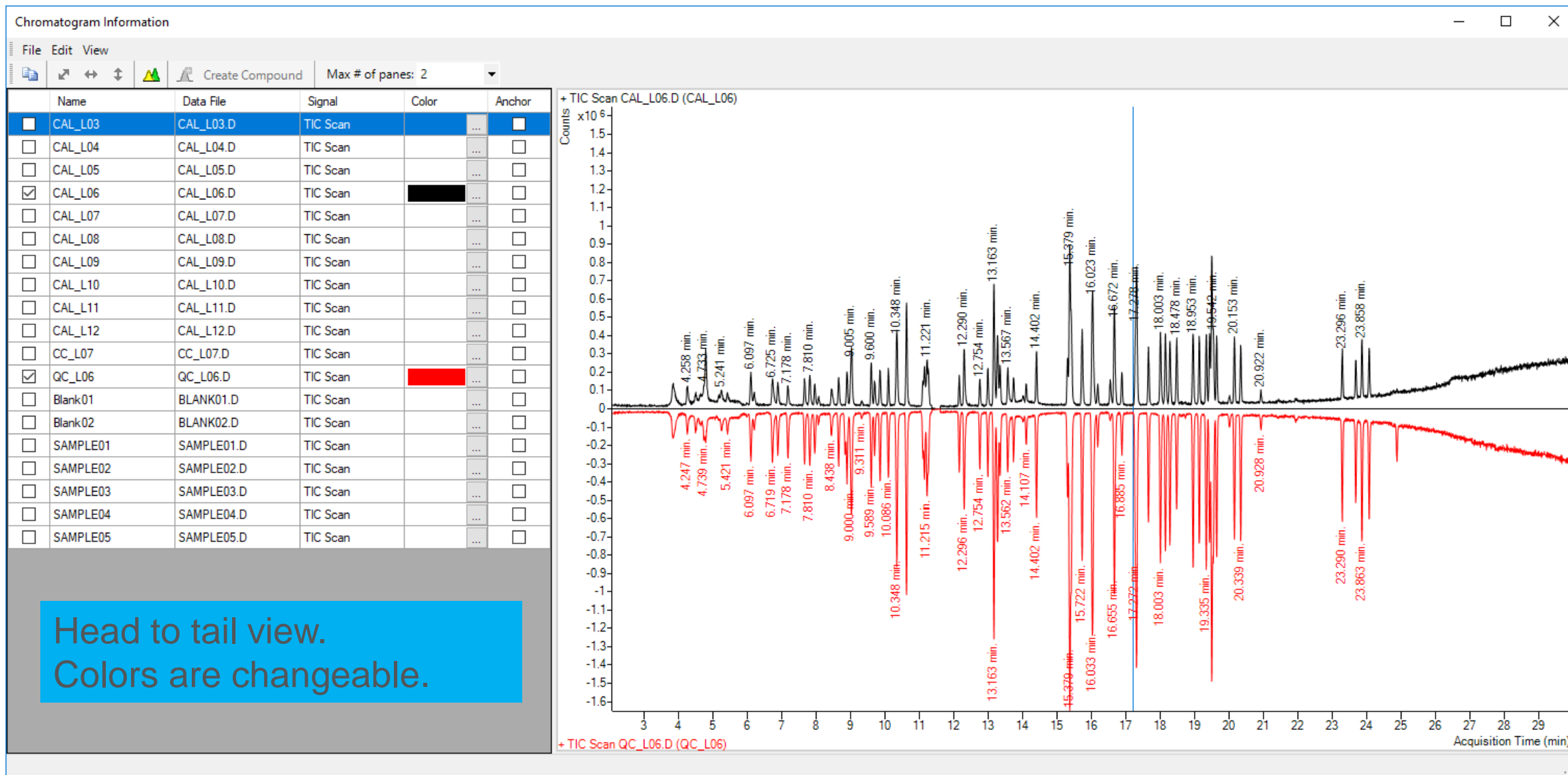
Data Review

Chromatogram Information



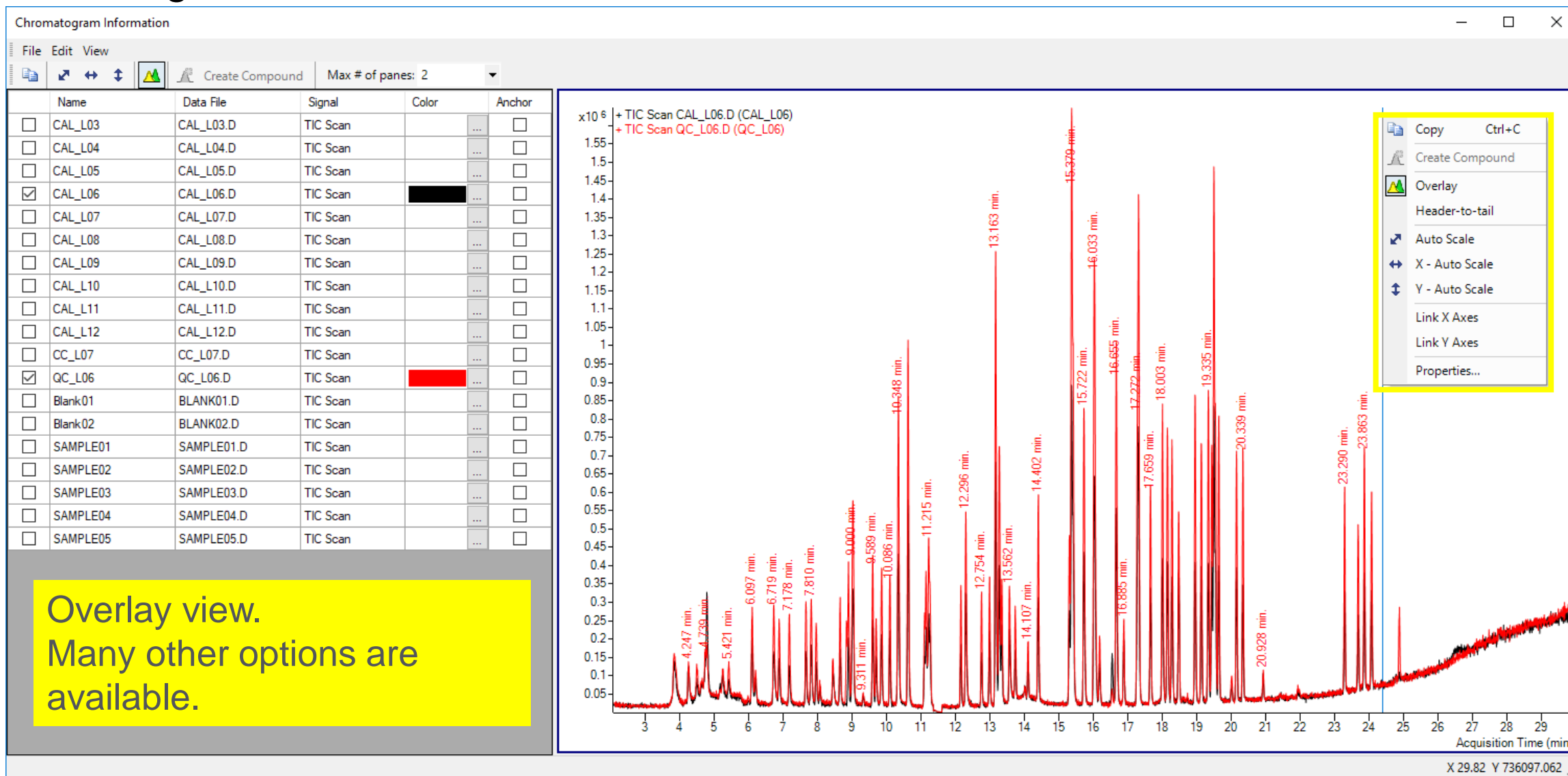
Data Review

Chromatogram Information



Data Review

Chromatogram Information



The screenshot displays the Agilent MassHunter Quantitative Analysis interface. The main window shows a data table with columns for Acq. Date-Time, Exp. Conc., RT, Resp., MI, Calc. Conc., Final Conc., Accuracy, Ratio, and Qualification. A 'Batch Table' sidebar is visible on the left. Below the table, there are several chromatograms and mass spectra plots. A 'Compound Information' sidebar is also present. At the bottom, an 'Auto Review' control panel is shown with buttons for Stop, Pause, Continue, and a variable interval setting.

| Sample | 1,1-Dichl... | 1,1-Dichloroethane Results | Qualifie.. | Qualifie.. | Fluorobenzene (L... | Qualifie.. | Qualifie.. |
|--------------------|--------------|----------------------------|------------|------------|---------------------|------------|----------------|
| 6/20/2008 11:53 AM | 0.5000 | 7.958 24856 | 0.8227 | 0.8227 | 164.5 | 39.7 | 10.621 1344085 |
| 6/20/2008 12:30 PM | 1.0000 | 7.952 49460 | 1.3069 | 1.3069 | 130.7 | 34.9 | 10.621 1180500 |
| 6/20/2008 1:06 PM | 2.0000 | 7.952 97828 | 2.2080 | 2.2080 | 110.4 | 33.3 | 10.621 1144972 |
| 6/20/2008 1:44 PM | 5.0000 | 7.958 152073 | 4.9316 | 4.9316 | 98.6 | 33.2 | 10.621 700572 |
| 6/20/2008 2:21 PM | 10.0000 | 7.958 520064 | 9.9799 | 9.9799 | 99.8 | 32.9 | 10.621 1128028 |
| 6/20/2008 3:04 PM | 15.0000 | 7.958 820986 | 14.6465 | 14.6465 | 97.6 | 33.6 | 10.621 1195789 |
| 6/20/2008 3:41 PM | 20.0000 | 7.958 1169293 | 19.8213 | 19.8213 | 99.1 | 32.8 | 10.621 1248377 |
| 6/20/2008 4:19 PM | 30.0000 | 7.952 1825977 | 29.2775 | 29.2775 | 97.6 | 32.7 | 10.621 1310216 |
| 6/20/2008 4:57 PM | 40.0000 | 7.958 2553725 | 39.5069 | 39.5069 | 98.8 | 33.5 | 10.626 1352603 |
| 6/20/2008 5:35 PM | 50.0000 | 7.958 3539675 | 50.9986 | 50.9986 | 102.0 | 33.5 | 10.621 1448684 |
| 6/20/2008 6:13 PM | 10.0000 | 7.952 615398 | 9.8424 | 9.8424 | 98.4 | 34.7 | 10.621 1354326 |
| 6/20/2008 6:50 PM | 5.0000 | 7.952 303201 | 5.3119 | 5.3119 | 106.2 | 35.0 | 10.620 1287756 |
| 6/20/2008 7:28 PM | | 7.947 26895 | 0.9033 | 0.9033 | | 33.2 | 10.626 1201125 |
| 6/20/2008 8:07 PM | | 8.667 666 | 0.4530 | 0.4530 | | 92.6 | 10.621 1056106 |
| 6/20/2008 8:44 PM | | 8.089 544 | 0.4497 | 0.4497 | | 16. | 10.621 1165447 |
| 6/20/2008 9:22 PM | | 8.640 334 | 0.4461 | 0.4461 | | 15. | 10.626 1138523 |
| 6/20/2008 10:00 PM | | 8.356 577 | 0.4515 | 0.4515 | | 10. | 10.621 1036288 |
| 6/20/2008 10:38 PM | | 8.258 232 | 0.4448 | 0.4448 | | 17. | 10.621 990498 |
| 6/20/2008 11:16 PM | | 7.958 745408 | 13.2332 | 13.2332 | | 34.5 | 10.621 1205652 |

Auto Review Samples

- Displays sample by sample.

Auto Review Compounds

- Displays compound by compound.

The 'Auto Review' control panel includes a close button (X), a 'Stop' button, a 'Pause' button, a 'Continue' button, and an 'Interval' field set to '5' with the unit 'sec'.

- Available in Flat Table or Compound Table.
- Stop, pause, continue and variable intervals.



Demo time

An **outlier** is a result that is outside the range of acceptable values for a given parameter.

What outliers are important in the workflow?

- Retention Time...
- Limit of Detection, Quantitation, Method Detection Limit.
- Qualifier Ratio.
- ISTD Response or ISTD Response Percent Deviation.
- QC, QC Relative Standard Deviation, QC LCS Recovery...
- CC, CC Average Response Factor, CC ISTD Response Ration...
- Matrix Spike, Matrix Spike Percent Recovery....

Outliers Setup Tasks

Method > Edit > Outlier Setup Tasks

Method Setup Tasks

- Compound Setup
- Retention Time Setup
- ISTD Setup
- Concentration Setup
- Qualifier Setup
- Calibration Curve Setup
- Globals Setup
- Save / Exit
- Manual Setup Tasks
- Outlier Setup Tasks**
- Retention Time



The screenshot displays the Agilent MassHunter software interface. The 'Method Tasks' sidebar on the left is highlighted with a purple border, and the 'Outlier Setup Tasks' option is selected. The main window shows a 'Method Table' with a table of samples and a 'Sample Information' section. Below this, there are two chromatograms: a Total Ion Chromatogram (TIC) and an Extracted Ion Chromatogram (EIC) for the peak at 4.248 minutes.

| Sample | Name | Data File | Type | Level | Acq. Method File | Acq. Date-Time |
|---------|-----------|-----------|------|--------|-------------------|----------------|
| CAL_L07 | CAL_L07.D | Cal | 7 | 624A.M | 6/20/2008 2:21... | |

| Quantifier | Name | TS | Scan | Type |
|----------------------|----------------------|----|------|--------|
| 1,1-Dichloro-1-pr... | 1,1-Dichloro-1-pr... | 1 | Scan | Target |
| Dichlorodifluoro... | Dichlorodifluoro... | 1 | Scan | Target |
| Chloromethane | Chloromethane | 1 | Scan | Target |
| 1,4-Dichloroben... | 1,4-Dichloroben... | 1 | Scan | Target |
| Vinyl Chloride | Vinyl Chloride | 1 | Scan | Target |
| 1,2,4-Trichlorob... | 1,2,4-Trichlorob... | 1 | Scan | Target |
| Bromomethane | Bromomethane | 1 | Scan | Target |

The chromatograms show 'Counts' on the y-axis and 'Acquisition Time (min)' on the x-axis. The TIC scan shows a complex pattern of peaks, while the EIC scan shows a single prominent peak at 4.248 minutes.

Outliers are setup in the Method Editor and are part of quantitation method.

Outliers Setup Tasks

~ 48 Outliers are available.










Outliers are not calculated unless values have been set up.






Outliers are used to perform automated quality checks.

Aids in data review by highlighting problem areas.

Increases confidence in data integrity by utilizing outliers.

Which outliers are important for my workflow?

| Outlier Setup Tasks | |
|---|---------------------------------|
|  | Retention Time |
| | Relative Retention Time |
| | Peak Resolution |
|  | Peak Symmetry |
| | Peak Full Width Half Maximum |
|  | Peak Purity |
| | Plates |
| | Capacity Factor |
|  | Signal-to-Noise Ratio |
|  | Limit Of Detection |
| | Limit Of Quantitation |
| | Method Detection Limit |
|  | Qualifier Ratio |
| | QValue |
| | Qualifier Coelution Score |
|  | ISTD Response |
| | ISTD Response Percent Deviation |
| | Sample Amount |
| | Sample RSD |
|  | Blank Concentration |
| | Blank Response |
| | Accuracy |
| | Average Response Factor |
| | Average Response Factor RSD |
|  | Curve Fit R2 |

| | Relative Response Factor |
|---|---------------------------------|
| | Response Factor |
|  | QC |
| | QC Relative Standard Deviation |
| | QC LCS Recovery |
|  | CC Average Response Factor |
| | CC ISTD Response Ratio |
| | CC Relative Response Factor |
| | CC Response Ratio |
| | CC Retention Time |
|  | Matrix Spike |
| | Matrix Spike Percent Difference |
| | Matrix Spike Percent Recovery |
| | Matrix Spike Group Recovery |
|  | Surrogate |
| | Surrogate Percent Recovery |
| | Response Check |
| | Mass Accuracy |
| | Mass Match Score |
|  | Library Match Score |
| | Alternative Peak |
| | Custom Calculation |
| Advanced Tasks | |

Outliers

- Most Outliers have both a low and high limit.
- Both limits need to be set for the outlier to be calculated.

| | |
|--|---------------------------------|
| | ISTD Response |
| | ISTD Response Percent Deviat... |
| | Sample Amount |
| | Sample RSD |
| | Blank Concentration |
| | Blank Response |
| | Accuracy |

| Quantifier | | | | | | |
|------------|----|----------------|------|--------|----------------------|-----------------------|
| Name | TS | Transition | Scan | Type | ISTD Resp. Limit Low | ISTD Resp. Limit High |
| ▶ Amp | 1 | 136.2 -> 91.4 | MRM | Target | | |
| Amp-d5 | 1 | 141.1 -> 93.4 | MRM | ISTD | | |
| Cocaine | 1 | 304.1 -> 182.0 | MRM | Target | | |
| Cocaine-d3 | 1 | 307.1 -> 185.0 | MRM | ISTD | | |
| MDMA | 1 | 194.2 -> 163.3 | MRM | Target | | |
| MDMA-d5 | 1 | 199.2 -> 164.3 | MRM | ISTD | | |
| Meth | 1 | 150.1 -> 119.3 | MRM | Target | | |
| Meth-d5 | 1 | 155.2 -> 92.3 | MRM | ISTD | | |

| | |
|--|------------------------|
| | Limit Of Detection |
| | Limit Of Quantitation |
| | Method Detection Limit |
| | Qualifier Ratio |
| | QValue |
| | Coelution Score |
| | ISTD Response |

| Quantifier | | | | | |
|------------|----|----------------|------|--------|-----|
| Name | TS | Transition | Scan | Type | LOD |
| ▶ Amp | 1 | 136.2 -> 91.4 | MRM | Target | |
| Amp-d5 | 1 | 141.1 -> 93.4 | MRM | ISTD | |
| Cocaine | 1 | 304.1 -> 182.0 | MRM | Target | |
| Cocaine-d3 | 1 | 307.1 -> 185.0 | MRM | ISTD | |
| MDMA | 1 | 194.2 -> 163.3 | MRM | Target | |
| MDMA-d5 | 1 | 199.2 -> 164.3 | MRM | ISTD | |
| Meth | 1 | 150.1 -> 119.3 | MRM | Target | |
| Meth-d5 | 1 | 155.2 -> 92.3 | MRM | ISTD | |

- Some outliers are one dimensional.
- A few only have a single limit.

Outliers

Batch Table



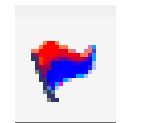
Icons on the toolbar.



Select Outliers



Turn off outlier filter



Display rows that have High/Low outliers



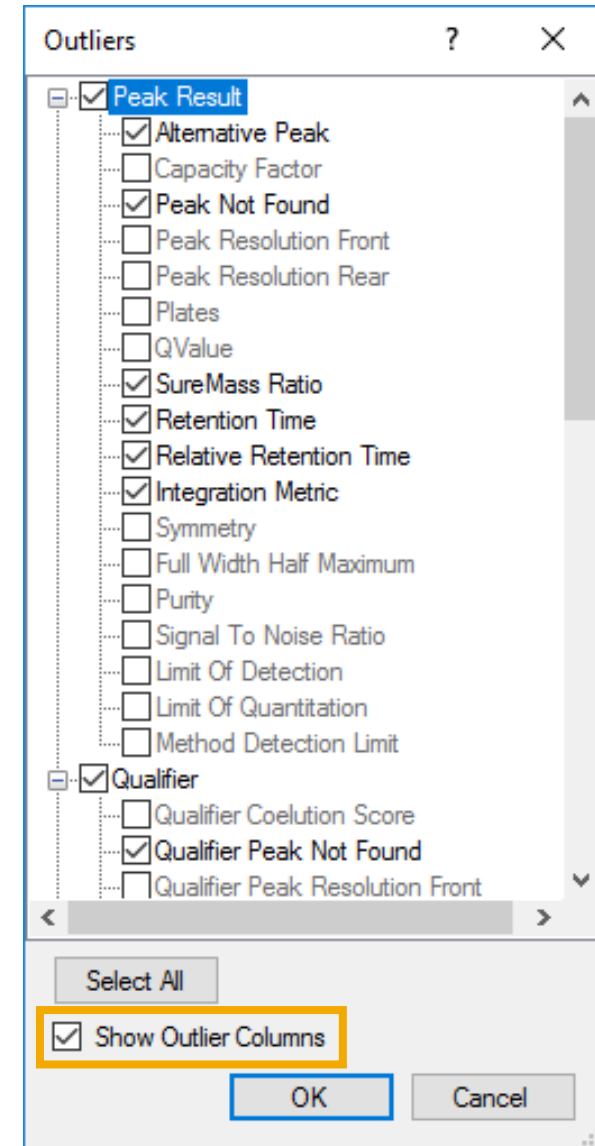
Display rows that have High outliers



Display rows that have Low outliers



Display rows that have no outliers



Outliers

Messages and Outliers

Batch Table

Sample: CAL_L10 Sample Type: <All> Compound: Dichlorodifluoromethane ISTD: Fluorobenzene

| Sample | | | | | | | Dichlorodifluoromethane Results | | | | | | | Fluorobenzene (L) | | Qualifie.. | | Qualifie.. | | |
|---------|-----------|-------|-------|--------------------|--------------|------------|---------------------------------|---------|----|-------------|-------------|----------|-------|-------------------|--------|------------|-------|------------|-------|----|
| Name | Data File | Type | Level | Acq. Date-Time | Sample Group | Exp. Conc. | RT | Resp. | MI | Calc. Conc. | Final Conc. | Accuracy | Ratio | MI | RT | Resp. | Ratio | MI | Ratio | MI |
| CAL_L03 | CAL_L03.D | Cal | 3 | 6/20/2008 11:53 AM | | 0.5000 | 4.237 | 29715 | | 0.4278 | 0.4278 | 85.6 | 33.6 | | 10.621 | 1344418 | 1.9 | | 9.5 | |
| CAL_L04 | CAL_L04.D | Cal | 4 | 6/20/2008 12:30 PM | | 1.0000 | 4.242 | 66597 | | 1.0238 | 1.0238 | 102.4 | 30.2 | | 10.621 | 1183924 | 1.8 | | 10.1 | |
| CAL_L05 | CAL_L05.D | Cal | 5 | 6/20/2008 1:06 PM | | 2.0000 | 4.247 | 127904 | | 1.9920 | 1.9920 | 99.6 | 31.6 | | 10.620 | 1144890 | 2.0 | | 10.5 | |
| CAL_L06 | CAL_L06.D | Cal | 6 | 6/20/2008 1:44 PM | | 5.0000 | 4.258 | 203734 | | 5.1178 | 5.1178 | 102.4 | 31.1 | | 10.621 | 700587 | 1.6 | | 9.8 | |
| CAL_L07 | CAL_L07.D | Cal | 7 | 6/20/2008 2:21 PM | | 10.0000 | 4.248 | 671861 | | 10.4356 | 10.4356 | 104.4 | 32.4 | | 10.621 | 1128268 | 2.0 | | 11.0 | |
| CAL_L08 | CAL_L08.D | Cal | 8 | 6/20/2008 3:04 PM | | 15.0000 | 4.242 | 1105069 | | 16.1636 | 16.1636 | 107.8 | 31.4 | | 10.621 | 1196415 | 2.0 | | 10.9 | |
| CAL_L09 | CAL_L09.D | Cal | 9 | 6/20/2008 3:41 PM | | 20.0000 | 4.242 | 1474827 | | 20.6623 | 20.6623 | 103.3 | 32.0 | | 10.620 | 1248377 | 2.0 | | 10.4 | |
| CAL_L10 | CAL_L10.D | Cal | 10 | 6/20/2008 4:19 PM | | 30.0000 | 4.248 | 2199968 | | 29.3491 | 29.3491 | 97.8 | 33.0 | | 10.621 | 1310216 | 1.7 | | 10.3 | |
| CAL_L11 | CAL_L11.D | Cal | 11 | 6/20/2008 4:57 PM | | 40.0000 | 4.247 | 3126148 | | 40.3840 | 40.3840 | 101.0 | 33.0 | | 10.626 | 1352547 | 1.9 | | 10.6 | |
| CAL_L12 | CAL_L12.D | Cal | 12 | 6/20/2008 5:35 PM | | 50.0000 | 4.247 | 3975819 | | 47.9439 | 47.9439 | 95.9 | 32.8 | | 10.621 | 1448684 | 2.1 | | 10.3 | |
| CC_L07 | CC_L07.D | CC | 7 | 6/20/2008 6:13 PM | | 10.0000 | 4.247 | 802673 | | 10.3859 | 10.3859 | 103.9 | 33.8 | | 10.621 | 1354419 | 1.6 | | 10.7 | |
| QC_L06 | QC_L06.D | QC | 6 | 6/20/2008 6:50 PM | | 5.0000 | 4.247 | 211200 | | 2.9037 | 2.9037 | 58.1 | 32.1 | | 10.620 | 1288192 | 1.7 | | 10.5 | |
| Blank01 | BLANK01.D | Blank | | 6/20/2008 7:28 PM | | | 4.258 | 20853 | | 0.3450 | 0.3450 | | 37.2 | | 10.626 | 1201381 | 2.1 | | 10.9 | |
| Blank02 | BLANK02.D | Blank | | 6/20/2008 8:07 PM | | | 4.630 | 266 | | 0.0464 | 0.0464 | | 163.6 | | 10.621 | 1059821 | 1.9 | | 10.3 | |

Select
Outliers
for Display

Red Outlier – High
(above upper limit)

Blue Outlier – Low
(below lower limit)



Messages

Quantitation Message(s)
 Dibromomethane: Qualifier M/Z = 93.0: Qualifier peak not found or does not match quantitation criteria
 Hexachlorobutadiene: Qualifier M/Z = 223.0: Qualifier peak not found or does not match quantitation criteria
 Hexachlorobutadiene: Qualifier M/Z = 227.0: Qualifier peak not found or does not match quantitation criteria
 Tetrahydrofuran: Qualifier M/Z = 72.0: Qualifier peak not found or does not match quantitation criteria
 Vinyl Acetate: Qualifier M/Z = 86.1: Qualifier peak not found or does not match quantitation criteria



Outliers

Outlier(s)
 Dichlorodifluoromethane: Retention time = 4.630 is outside the allowed range [4.037, 4.462]

Hover cursor over the outlier or message to display details

Outliers

Filter on Outliers in Batch Table

Agilent MassHunter Quantitative Analysis (for GCMS) - VOA - VolatileOrganics.batch.bin

File Edit View Analyze Method Update Library Report Tools Help

Analyze Batch ▾ Layout: [Icons] Restore Default Layout

Batch Table

Sample: Blank02 Sample Type: <All> Compound: 1,1,1-Trichloroethane ISTD: Fluorobenzene

| Sample | | | | | | 1,1,1-Trichloroethane Results | | | | | | Qualifier (9... | | Qualifier (...) | | Fluorobenzene (L... | | Qualifie... | | Qualifie... | | | |
|--------|---|----------|------------|--------|-------|-------------------------------|------------|--------|-------|----|-------------|-----------------|----------|-----------------|----|---------------------|----|-------------|---------|-------------|------|-------|----|
| ? | ▼ | Name | Data File | Type | Level | Acq. Date-Time | Exp. Conc. | RT | Resp. | MI | Calc. Conc. | Final Conc. | Accuracy | Ratio | MI | Ratio | MI | RT | Resp. | Ratio | MI | Ratio | MI |
| | ▼ | Blank02 | BLANK02.D | Blank | | 6/20/2008 5:07 PM | | 10.370 | 313 | | 0.1851 | 0.1851 | | 21731.3 | | 5106.7 | | 10.621 | 1059821 | | 10.3 | | |
| | ▼ | SAMPLE02 | SAMPLE02.D | Sample | | 6/20/2008 6:22 PM | | 9.344 | 384 | | 0.1862 | 0.1862 | | | | 1831.1 | | 10.626 | 1120031 | 2.2 | | 10.8 | |
| | ▼ | SAMPLE04 | SAMPLE04.D | Sample | | 6/20/2008 7:38 PM | | 10.768 | 359 | | 0.1869 | 0.1869 | | 17099.9 | | 4476.3 | | 10.621 | 990498 | 2.5 | | 11.8 | |

Outliers

- Peak Result
 - Peak Not Found
 - Peak Resolution Front
 - Peak Resolution Rear
 - Retention Time
 - Relative Retention Time
 - Integration Metric
 - Symmetry
 - Full Width Half Maximum
 - Purity
 - Signal To Noise Ratio
 - Limit Of Detection
 - Limit Of Quantitation
 - Method Detection Limit
- Qualifier
 - Qualifier Peak Not Found

Select All

Show Outlier Columns

OK Cancel

By default all outliers are displayed but it is possible to limit this to a subset or single outlier for a more targeted data review pass.

Remember, an outlier is not active unless a limit has been specified for it in the Method Editor.

Outliers

Default outliers

| Outlier | Associated Column/Table | Comment |
|--------------------------------------|---|---------------------------------------|
| Integration Quality Metric | IntegrationMetricQualityFlags (Peak table) | Defaulted: Using Agile2 Integrator |
| Qualifier Integration Quality Metric | IntegrationMetricQualityFlags (PeakQualifier table) | Defaulted: Using Agile2 Integrator |
| Accuracy | Accuracy | Defaulted: +/-20% |
| Qualifier Ratio | QualifierResponseRatio (PeakQualifier) | Defaulted: +/- 20% |
| RetentionTime | RetentionTime | Defaulted: +/- 5% relative |
| Relative Retention Time | RetentionTime | Defaulted: +/- 10% relative |

By default these outliers are enabled.

If an outlier is not enabled, it is not calculated.

$$\text{Accuracy} = \text{Calculated/Expected} \times 100$$

New Feature - Help in HTML Format.

The screenshot shows a web browser window displaying the Agilent MassHunter Quantitative Analysis help page for Outliers. The browser address bar shows the file path: file:///C:/Program%20Files/Agilent/MassHunter/Workstation/Quant/help/en-US/QuantAnalysis/Classic/index.htm#t=c. The page title is "Agilent | MassHunter Quantitative Analysis". The navigation menu includes Home, Getting Started, Quantitative Analysis, Method Development, Outliers (highlighted with a red box), Reports, and Reference. The left sidebar lists various topics under "Outliers", including Outlier details, Outliers enabled by default, Display outlier monitored columns in the batch table, Peak result, Qualifier, ISTD, Sample, Blank, Calibration, QC, CC, Matrix, Surrogate, Response check, Mass, and Custom. The main content area is titled "Outliers" and contains the following text:

An outlier is a result value that is outside the range of acceptable values for that parameter as required by your protocol. The program allows you to choose the outliers that you want to show in your analyzed batch and set their limits using the **Outlier Method Tasks** menu in the **Method Edit** view.

Outlier messages displayed in the Batch Table are based on full precision of values. Values outside of the acceptable range may not be apparent in flagged outlier messages in cases where less precision is displayed.

For some outliers, when a primary peak is not found the compound and its containing sample will be flagged with a quantitation message, not with an outlier flag. For a list of outliers where peaks not found are handled this way see [Outlier Details](#).

At the bottom of the page, the date "18-Oct-2017" and the Agilent Technologies logo are visible, along with the copyright notice "© 2017 Agilent. All Rights Reserved".

Many Outliers also have Quant videos.

Name

- Outlier Criteria Intersection.mp4
- Outliers - Continuing Calibration - CC - Advanced.mp4
- Outliers - FWHM Chromatography - Advanced.mp4
- Outliers - Laboratory Control Spike - Advanced.wmv
- Outliers - Library Match Score - Advanced.wmv
- Outliers - Mass Accuracy - Advanced.wmv
- Outliers - Matrix Spike - Advanced.mp4
- Outliers - Matrix Spike - Introduction - Advanced.wmv
- Outliers - Matrix Spike Demo - Advanced.wmv
- Outliers - Matrix Spike Group Recovery Demo - Advanced.wmv
- Outliers - Matrix Spike Percent Difference Demo - Advanced.wmv
- Outliers - Matrix Spike Percent Recovery Demo - Advanced.wmv
- Outliers - Peak Not Found - Advanced.wmv
- Outliers - Peak Purity - Advanced.wmv
- Outliers - Pharma suitability - Advanced.mp4
- Outliers - Symmetry - Starter.mp4
- Outliers - Symmetry Demo - Starter.mp4

Metric Plot

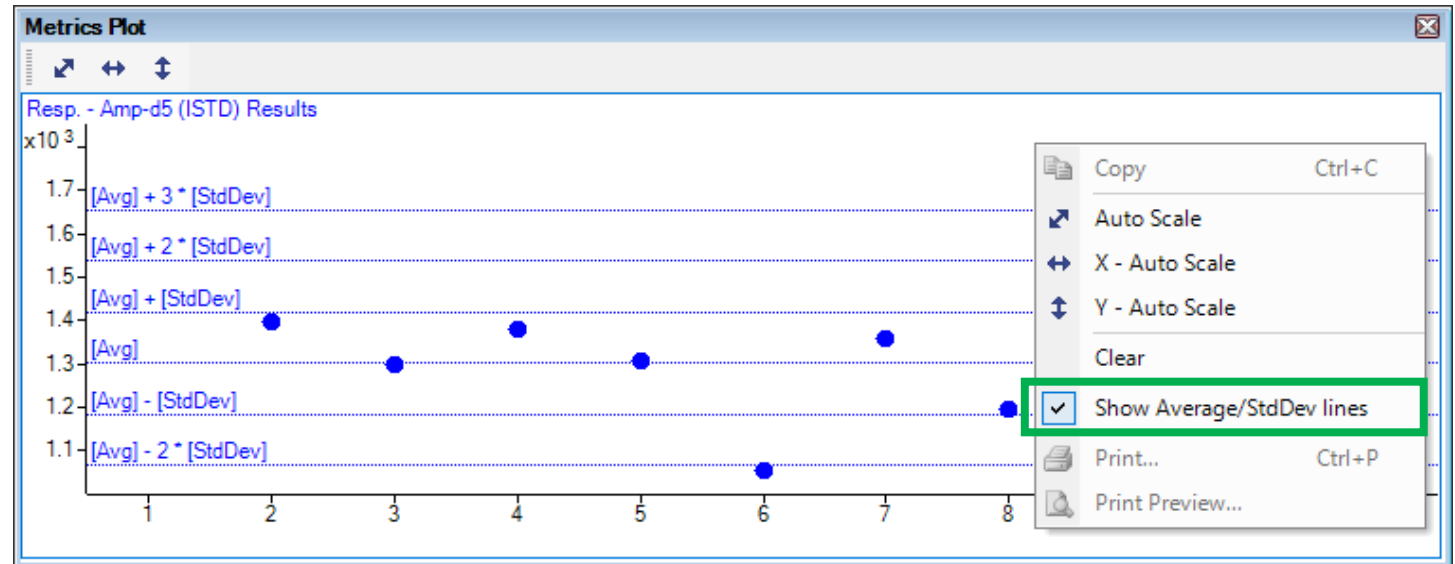
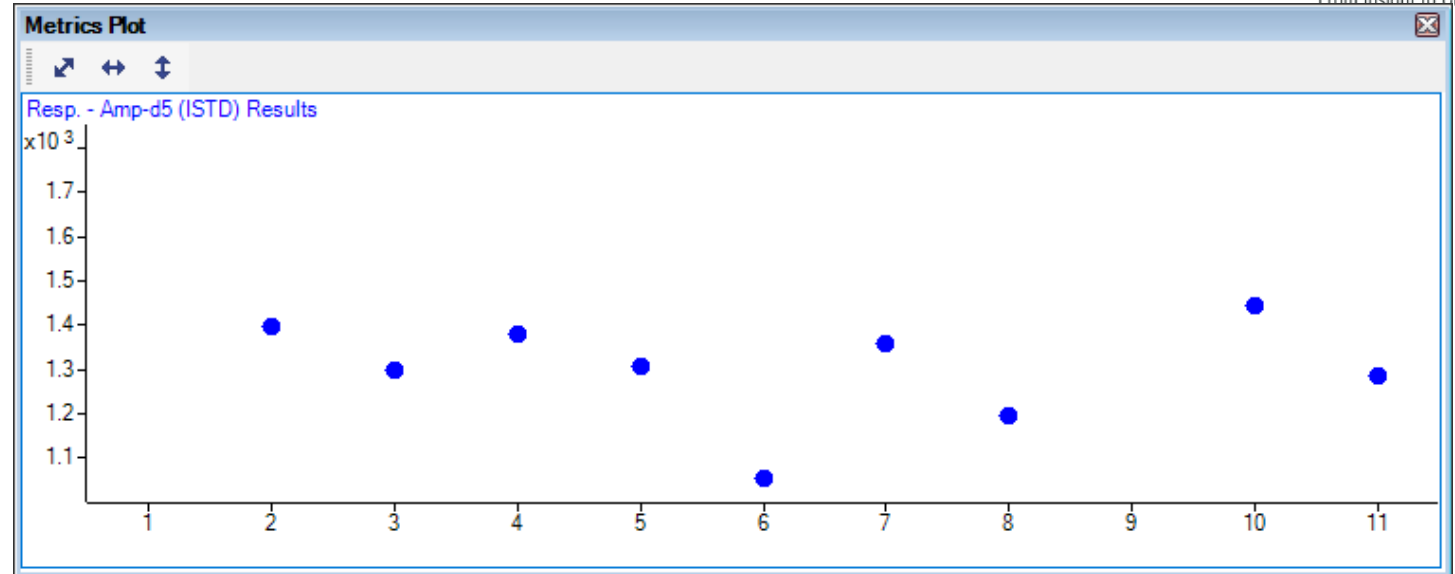
Right click (on header) > Plot this Column.

| Amp-d5 (ISTD) Results | |
|-----------------------|-------|
| RT | Resp. |
| 2.129 | 1397 |
| 2.128 | 1298 |
| 2.121 | 1377 |
| 1.990 | 1304 |
| 2.076 | 1053 |
| 2.131 | 1356 |
| 2.121 | 1196 |
| 2.130 | 1445 |
| 2.089 | 1284 |

- Add/Remove Columns...
- Add Column
- Remove Column
- Restore Default Columns
- Auto Fit Columns Ctrl+U
- Format Column...
- Reset Sort
- Lock Sample/Compound Columns
- Plot this Column

Right click (in the plot window) > Show Average/Std Dev lines.

Tip: Use Metric Plot for determining potential problems.



Compounds at a Glance

View > Compounds-at-a-Glance

Custom layouts can be loaded and saved.

Agilent MassHunter Quantitative Analysis (for GCMS) - Wayne MH TD Data - Wayne_TD_with_deconv_CAS_num

File Edit View Analyze Method Update Report Tools Help

Batch Table Compound Information

Batch Table Calibration Curve

Sample: Sample Type: <All> Comp

| Acq. Date-Time | RT | RT | Resp | MI | Ca |
|-----------------|--------|--------|--------|----|----|
| 7/2012 11:36 PM | 12.429 | 12.544 | 679 | | |
| 8/2012 12:20 AM | 12.429 | 12.393 | 878 | | |
| 8/2012 1:05 AM | 12.429 | 12.472 | 1883 | | |
| 8/2012 1:50 AM | 12.429 | 12.465 | 1018 | | |
| 8/2012 2:35 AM | 12.429 | 12.435 | 15317 | | |
| 8/2012 3:19 AM | 12.429 | 12.502 | 20987 | | |
| 8/2012 4:04 AM | 12.429 | 12.441 | 823 | | |
| 8/2012 4:49 AM | 12.429 | 12.381 | 1266 | | |
| 8/2012 5:35 AM | 12.429 | 12.465 | 2002 | | |
| 8/2012 6:18 AM | 12.429 | 12.453 | 1026 | | |
| 8/2012 7:02 AM | 12.429 | 12.441 | 7355 | | |
| 8/2012 7:47 AM | 12.429 | 12.472 | 2342 | | |
| 8/2012 8:31 AM | 12.429 | 12.455 | 2699 | | |
| 8/2012 9:16 AM | 12.429 | 12.453 | 1902 | | |
| 8/2012 10:00 AM | 12.429 | 12.471 | 2327 | | |
| 8/2012 10:44 AM | 12.429 | 12.478 | 4735 | | |
| 8/2012 11:29 AM | 12.429 | 12.508 | 41423 | | |
| 8/2012 12:13 PM | 12.429 | 12.417 | 123626 | | |
| 8/2012 12:58 PM | 12.429 | 12.429 | 4505 | | |
| 8/2012 1:42 PM | 12.429 | 12.423 | 4030 | | |
| 8/2012 2:27 PM | 12.429 | 12.423 | 1200 | | |
| 8/2012 3:11 PM | 12.429 | 12.356 | 905 | | |

View > **Compounds-at-a-Glance...**

Compounds at a Glance

File Edit View Layout Help

- Samples/Targets/Auto Scale
- Samples/Targets/Link X Axes + Fit to low CAL
- Samples/Targets/Overlay Qualifiers + Link X Axes
- Samples/Targets/Overlay ISTDs + Link X, Y Axes
- Samples/ISTDs/Overlay Qualifiers + Link X Axes
- Samples/Targets/By Compound Wrapped + Fit to low CAL
- Samples/Targets/By Sample Wrapped + Fit to low CAL
- Setup...
- Load Layout...**
- Save Layout...



Compounds at a Glance

The image shows three overlapping 'Setup Graphics' dialog boxes. The top-left one is on the 'Samples' tab, the middle one is on the 'Compounds' tab, and the bottom one is on the 'Organize' tab. The 'Organize' tab shows options for 'Organize Rows by' (Samples, Compounds, Qualifiers), 'Overlay' (Qualifiers, ISTD, Matrix Spike, etc.), 'Review Mode' (None, Sample by Sample, Compound by Compound), and 'Display Options' (Wrap Rows, Baselines, Fill Peaks, etc.).

The fourth dialog box on the right is on the 'Outlier' tab. It shows a list of qualifiers with checkboxes. A blue box highlights the 'Filter' section at the bottom, which contains three radio button options: 'Show all panes', 'Show panes without outliers' (which is selected), and 'Show panes with outliers'. A blue arrow points from the 'Organize' tab of the middle dialog box to this 'Filter' section.

| Name | Data File |
|-------------------------|------------|
| 1ul Splitless inject... | 10RLMTX.D |
| 1ul Splitless inject... | 5RLMTX.D |
| 1ul Splitless inject... | C3010795.D |
| 1ul Splitless inject... | C3010788.D |
| 1ul Splitless inject... | C3010800.D |
| Standard Mix a 1... | STD_AD |

| Name | Type |
|---------------------|--------|
| Diethylene glycol | Target |
| Aniline | Target |
| Phenol | Target |
| 2-Chlorophenol | Target |
| 1,3-Dichlorobenzene | Target |
| p-Dichlorobenzene | Target |
| Dicyclopentadiene | Target |

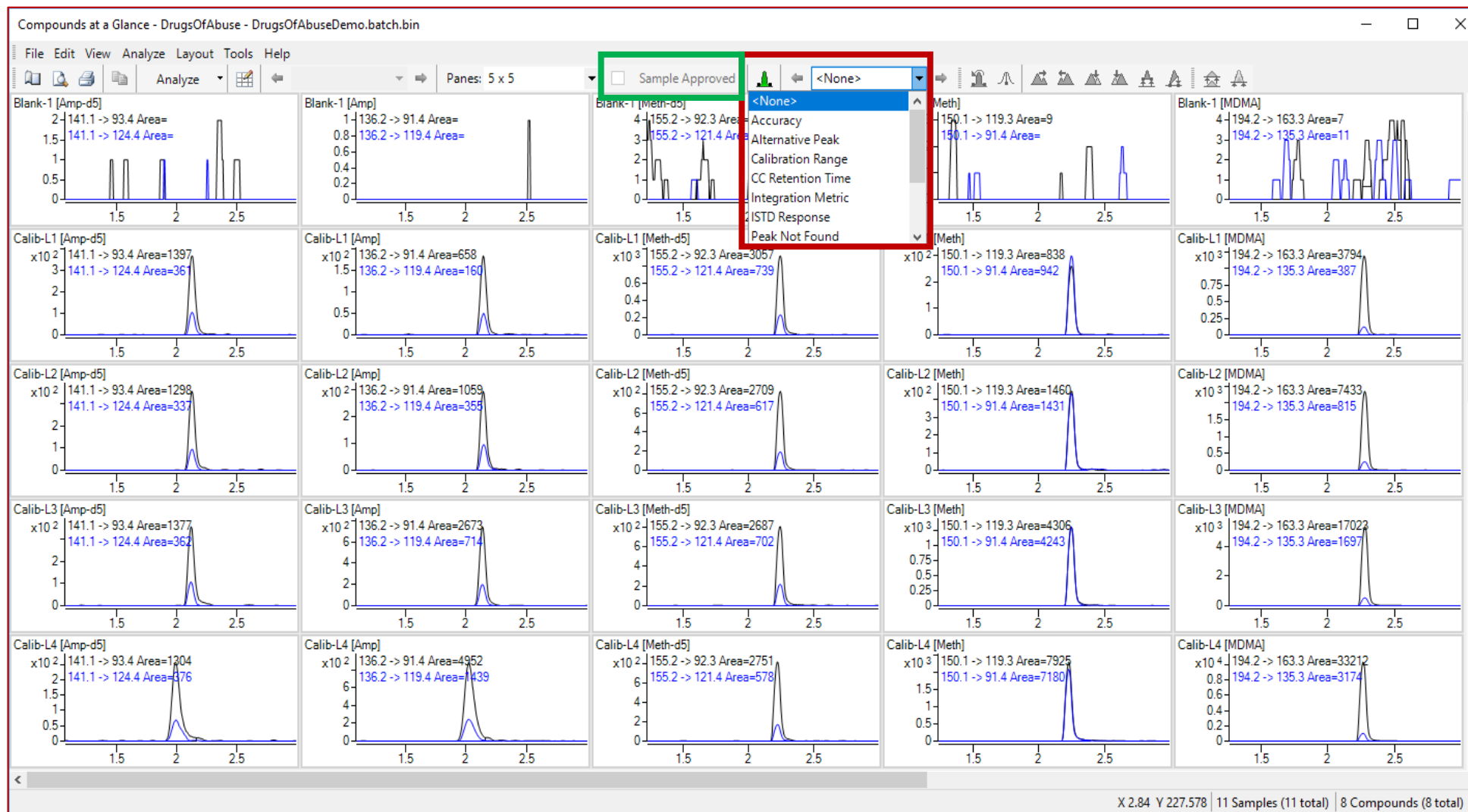
- Peak Result
 - Peak Not Found
 - Peak Resolution Front
 - Peak Resolution Rear
 - Retention Time
 - Relative Retention Time
 - Integration Metric
 - Symmetry
 - Full Width Half Maximum
 - Purity
 - Signal To Noise Ratio
 - Limit Of Detection
 - Limit Of Quantitation
 - Method Detection Limit
- Qualifier
 - Qualifier Peak Not Found
 - Qualifier Peak Resolution Front
 - Qualifier Peak Resolution Rear
 - Qualifier Signal To Noise Ratio
 - Qualifier Ratio
 - Qualifier Integration Metric
 - Qualifier Peak Symmetry
 - Qualifier Peak Full Width Half Maximum
- ISTD
- Sample
- Blank
- Calibration
 - Average Response Factor RSD

Filter:

- Show all panes
- Show panes without outliers
- Show panes with outliers

Layout > Setup Layout
Select various Qualifiers
Show panes with or without outliers

Compounds at a Glance Data Review



Sample Approved
box for QA.

Display outliers by
category.

New Feature in
Quant B.09.00

Compounds at a Glance

Review Sample by Sample

- Can be reviewed Sample by Sample.
- Optional Pane Dimensions
- Can scroll through the samples.
- Once the layout is saved it can be loaded time after time.
- Numerous Predefined Layouts

| |
|---|
| Samples/Targets/Auto Scale |
| Samples/Targets/Link X Axes + Fit to low CAL |
| Samples/Targets/Overlay Qualifiers + Link X Axes |
| Samples/Targets/Overlay ISTDs + Link X, Y Axes |
| Samples/ISTDs/Overlay Qualifiers + Link X Axes |
| Samples/Targets/By Compound Wrapped + Fit to low CAL |
| Samples/Targets/By Sample Wrapped + Fit to low CAL |
| Calibration/Targets/ByCompound Overlapped + Fit to peak |
| Calibration/ISTDs/ByCompound Overlapped + Fit to peak |

Setup Graphics

Samples | Compounds | **Organize** | Outlier

Organize Rows by:
 Compounds
 Samples

Review Mode
 None
 Sample by Sample
 Compound by Compound
 Compound Group by Compound Group

Overlay:
 None - target only
 None - target and qualifiers
 Qualifiers
 ISTD
 Matrix Spike
 Compound Groups
 Sample Groups
 Compounds
 Samples

Pane Dimension
3 x 2

Display Options
 Wrap Rows
 Baselines
 Fill Peaks
 Normalize
 Uncertainty Band

Peak Annotations

Area
 Calc. Conc.
 Final Conc.
 RT
 Height
 Ratio
 Delta RT
 S/N
 Q. Computed

Display annotation names (ex. RT=2.452)
 Display units for Conc., RT and Delta RT


Response ratio label:
Ratio

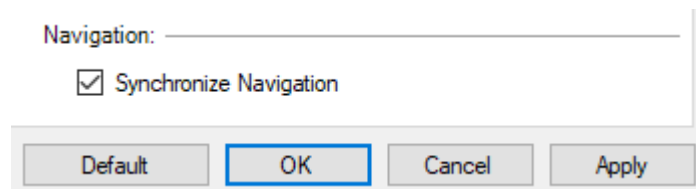
OK Cancel

< Back Next > Apply OK Cancel

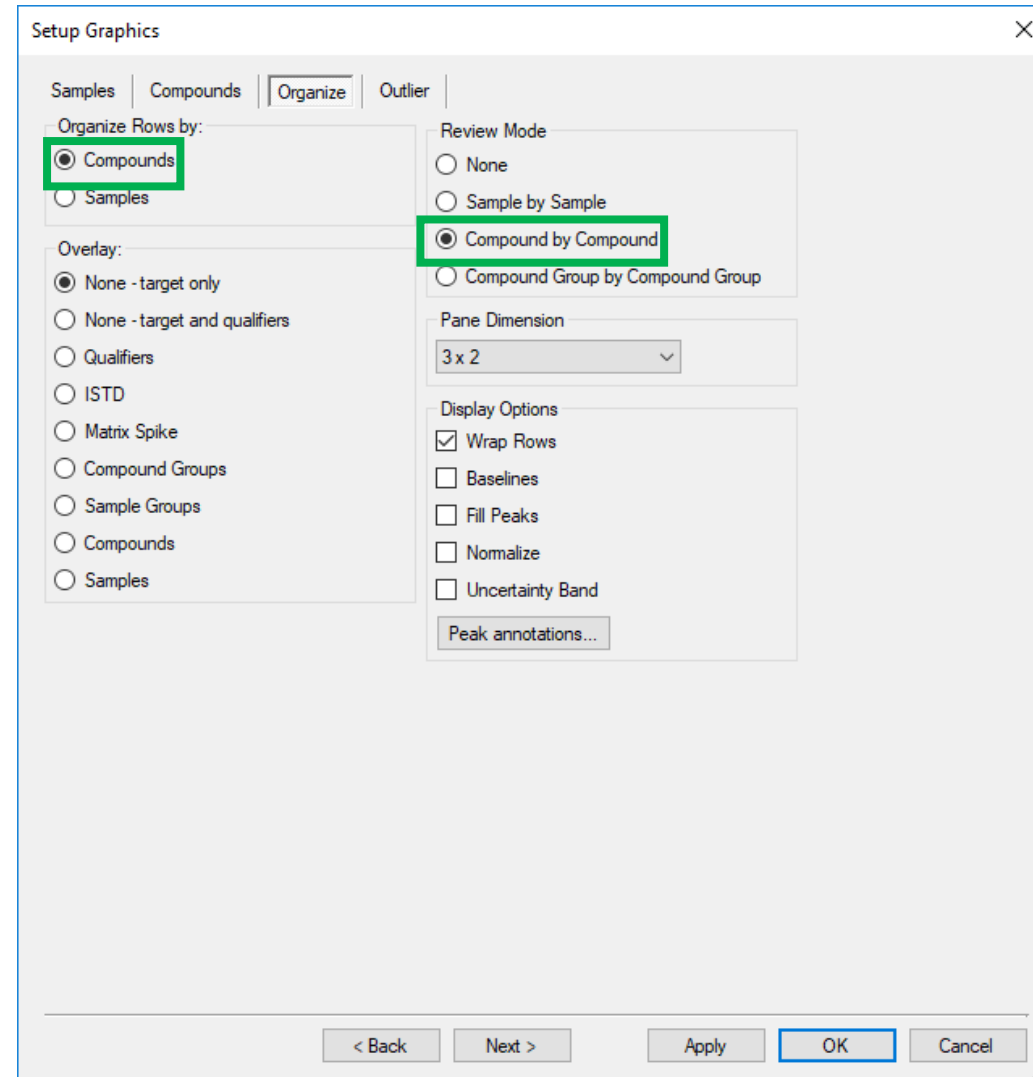
Compounds at a Glance

Review Compound by Compound

- Layout > Setup Layout or from 
- Layouts can be customized.
- Can be reviewed Compound by Compound.
- Various Overlay modes.
- Various Display Options.
- Can synchronize Compounds at a Glance with Quantitative Analysis.



- Right click **Properties > Synchronize Navigation** (global parameter).





Demo time

Summary

- Target Compound Analysis
- Quant Method Checklist
 - RT setup and RT Criteria
 - Reference and Non-Reference windows
- Integrators
 - Peak Filters
 - Adjusting Peak Filter Area Thresholds Zero Peak Below LOD
 - Correlation window
- Data Review
 - Filtering on Sample Type, Sample Group and Auto Review
- Outliers
 - ~ 48 outliers are available
 - Which outliers are important to my workflow?
- Compounds at a Glance
 - Display outliers by category.

Training Resources

Available Training Resources

Convenient Training

In our classrooms, at your site or online.

From a team of industry experts that deliver a high quality learning experience.

Classroom Training

Introductory level to in-depth, hands-on for laboratory instrumentation and software.

Customized On-Site Training

Effective learning environment designed to achieve operational excellence and employ development without the need to travel.

Online

Offerings from foundation level to expert delivered at your own pace.

Agilent University

Access From Home Page

Upgraded customer experience

Search and find courses that meet your interests and needs in the format they require.

Introduce new eLearning capabilities

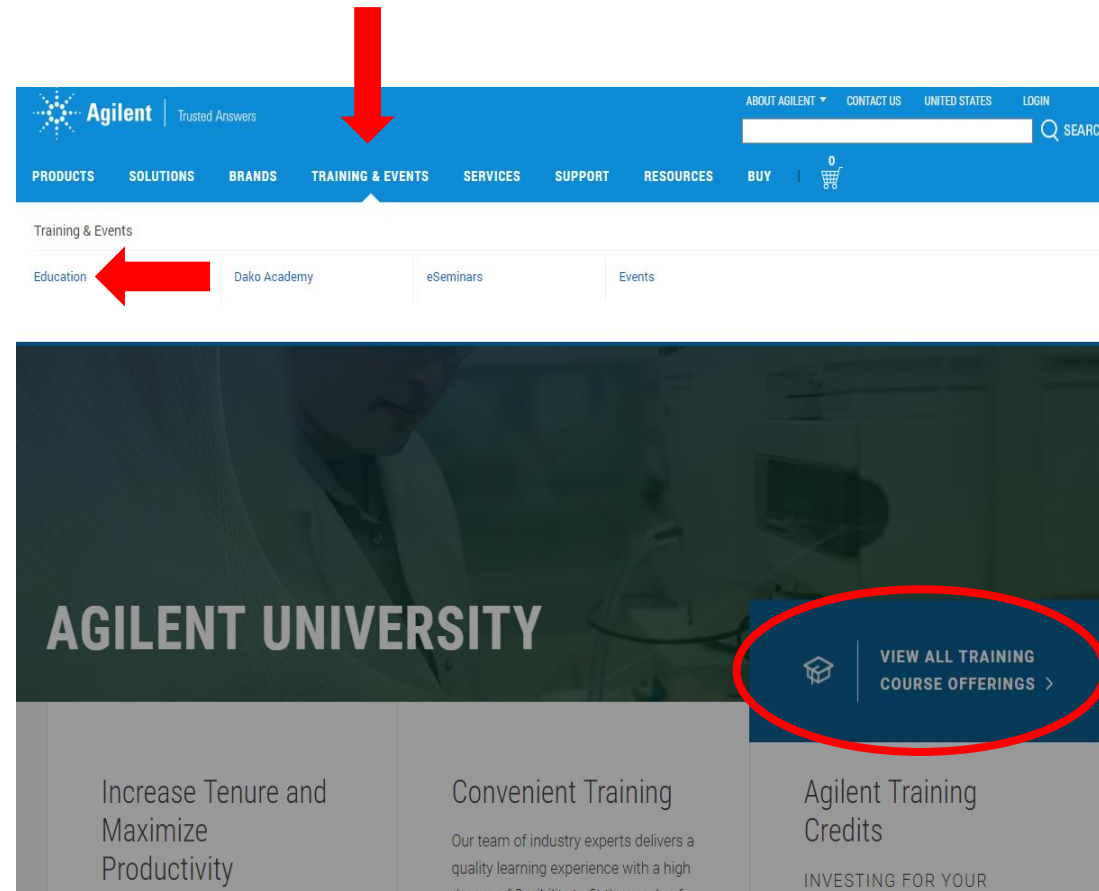
Recorded and video-based learning
Virtual online classes

Expanded portfolio

Foundational subjects
Intermediate subjects
Advanced subjects
Workflow and applications

Helping customers

Educate your employees on Agilent instruments and software.
From new hires to the most seasoned scientists.



Agilent Community



Collaborate - Ask and answer questions.

Connect - Interact with other Agilent users.

Discover - Find relevant discussions, documents, and videos.

Share - Contribute your insights.

